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The Surface Site Interaction Point Approach to Non-Covalent Interactions

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Contents

1 Experimentally Measured Solvent Parameters

Solvent	Canonical Smiles	InChIKey	$\alpha_{\mathbf{S}}$	$\beta_{\mathbf{S}}$	References
carbon tetrachloride	ClC(Cl)(Cl)Cl	VZGDMQKNWNREIO-UHFFFAOYSA-N	1.4	0.6	(*1*)
perfluoro-n-hexane	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	ZJIJAJXFLBMLCK-UHFFFAOYSA-N	1.2	0.3	(*2*)
benzene	c1ccccc1	UHOVQNZJYSORNB-UHFFFAOYSA-N	1.1	1.6	(*2*)
chlorobenzene	Clc1ccccc1	MVPPADPHJFYWMZ-UHFFFAOYSA-N	1.4	1.1	(*2*)
o-dichlorobenzene	Clc1ccccc1Cl	RFFLAFLAYFXFSW-UHFFFAOYSA-N	1.5	0.9	(*2*)
dichloromethane	ClCCl	YMWUJEATGCHHMB-UHFFFAOYSA-N	1.7	1.5	(*2*)
1,2-dichloroethane	ClCCCl	WSLDOOZREJYCGB-UHFFFAOYSA-N	1.7	1.6	(*2*)
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	UOCLXMDMGBRAIB-UHFFFAOYSA-N	1.3	1.3	(*2*)
chloroform	ClC(Cl)Cl	HEDRZPFGACZZDS-UHFFFAOYSA-N	2.2	1.3	(*3*) (*4*)
acetonitrile	CC#N	WEVYAHXRMPXWCK-UHFFFAOYSA-N	1.5	5.1	(*4*)
acetone	CC(C)=O	CSCPPACGZOOCGX-UHFFFAOYSA-N	1.2	5.7	(*5*)
alkanes			1.2	0.6	(*2*)
alkylalcohols			3.5	6.9	(*6*)

2 Experimentally Measured Solute α Parameters

2.1 CH HYDROGEN

2.1.1 HALOALKANE

Common Name	Canonical Smiles	InChIKey	α	References
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	UOCLXMDMGBRAIB-UHFFFAOYSA-N	1.4	(*7*)
1,2-dichloro-1,2-difluoroethane	F[C@@H](Cl)[C@H](F)Cl	IDSKMUOSMAUASS-XIXRPRMCSA-N	1.7	(*7*)
1,2-dichloroethane	ClCCCl	WSLDOOZREJYCGB-UHFFFAOYSA-N	1.7	(*7*)
1,2-dibromo-1,1-difluoroethane	FC(F)(Br)CBr	DPOZWTRVXPUOQW-UHFFFAOYSA-N	1.9	(*7*)
bromo(dichloro)methane	ClC(Cl)Br	FMWLUWPQPKEARP-UHFFFAOYSA-N	1.9	(*7*)
dichloromethane	ClCCl	YMWUJEATGCHHMB-UHFFFAOYSA-N	1.9	(*7*)(*8*)(*9*)
2,2-dichloro-1,1-difluoro-1-methoxy ethane	COC(F)(F)C(Cl)Cl	RFKMCNOHBTXSMU-UHFFFAOYSA-N	2.0	(*7*)
bromoform	BrC(Br)Br	DIKBFYAXUHHXCS-UHFFFAOYSA-N	2.1	(*7*)
1,2-dichloro-1-fluoroethane	F[C@@H](Cl)CCl	NDKGUMMLYBINOC-UWTATZPHSA-N	2.1	(*7*)
1-chloro-1,1,2-trifluoro-2-iodoethane	F[C@H](I)C(F)(F)Cl	XONGRFUEHPBOBB-PVQJCKRUSA-N	2.1	(*7*)
1,2,2-trichloro-1,1-difluoroethane	FC(F)(Cl)C(Cl)Cl	FQAMAOOEZDRHHB-UHFFFAOYSA-N	2.2	(*7*)
trichloro(2 h)methane	ClC(Cl)Cl	HEDRZPFGACZZDS-UHFFFAOYSA-N	2.2	(*7*)
1-bromo-2-chloro-1,1,2-trifluoroethane	F[C@@H](Cl)C(F)(F)Br	KFTODZKBBUMDQB-PVQJCKRUSA-N	2.2	(*7*)
chloroform	ClC(Cl)Cl	HEDRZPFGACZZDS-UHFFFAOYSA-N	2.2,2.1	(*7*)(*10*)(*8*)(*9*)
2-bromo-2-chloro-1,1,1-trifluoroethane	FC(F)(F)[C@@H](Cl)Br	BCQZXOMGPXTTIC-PVQJCKRUSA-N	2.3	(*7*)
2-chloro-1-(difluoromethoxy)-1,1,2-trifluoroethane	FC(F)OC(F)(F)[C@H](F)Cl	JPGQOUSTVILISH-SFOWXEAESA-N	2.1	(*7*)

2.1.2 X-CH HYDROGEN

Common Name	Canonical Smiles	InChIKey	α	References
propiononitrile	CCC#N	FVSKHRXBFJPNKK-UHFFFAOYSA-N	2.7	(*7*)
1,1-dinitroethane	CC([N+](=O)[O-])[N+](=O)[O-]	LKKHEZBRRGJBGH-UHFFFAOYSA-N	3.0	(*7*)
(e)-1,2-dichloroethene	Cl/C=C/Cl	KFUSEUYYWQURPO-OWOJBTEDSA-N	1.8	(*7*)

2.1.3 ALKYNE

Common Name	Canonical Smiles	InChIKey	α	References
heptyne	C#CCCCCC	YVXHZKKCZYLQOP-UHFFFAOYSA-N	1.7	(*11*)
n"-ethyl-n,n,n',n'-tetramethyl-n" -prop-2-ynyl-phosphoric triamide	C#CCN(CC)P(=O)(N(C)C)N(C)C	DETZZVPMDQPJIC-UHFFFAOYSA-N	1.8	(*7*)
N/A	C#CCN(CC)P(=O)(N(C)C)N(C)C	DETZZVPMDQPJIC-UHFFFAOYSA-N	1.8	(*11*)
but-3-ynyl bis(dimethylamino)phosphinate	C#CCCOP(=O)(N(C)C)N(C)C	GYHSJCJMDZRRJG-UHFFFAOYSA-N	1.9	(*11*)
prop-2-ynyl bis(diethylamido)phosphinate	C#CCOP(=O)(N(CC)CC)N(CC)CC	DEHSPEZTBSYMPL-UHFFFAOYSA-N	1.9	(*7*)
3,3-dimethyl-1-butyne	C#CC(C)(C)C	PPWNCLVNXGCGAF-UHFFFAOYSA-N	1.9	(*7*)
prop-2-ynyl bis(piperidino)phosphinate	C#CCOP(=O)(N1CCCCC1)N1CCCCC1	RVDBZQDTMHPUAJ-UHFFFAOYSA-N	1.9	(*7*)
prop-2-ynyl bis(diethylamido)phosphinate	C#CCP(=O)(N(CC)CC)N(CC)CC	VAFQAOSMSGEURX-UHFFFAOYSA-N	1.9	(*7*)
prop-2-ynyl bis(piperidino)phosphinate	C#CCOP(=O)(N1CCCCC1)N1CCCCC1	RVDBZQDTMHPUAJ-UHFFFAOYSA-N (	1.9	(*11*)
n-methyl n-propargyl bis-dimethylphosphoramide	C#CCN(C)P(=O)(N(C)C)N(C)C	DOYODMYEMDHHCE-UHFFFAOYSA-N	1.9	(*11*)
but-3-ynyl bis(dimethylamido)phosphinate	C#CCCOP(=O)(N(C)C)N(C)C	GYHSJCJMDZRRJG-UHFFFAOYSA-N	1.9	(*7*)
prop-2-ynyl bis(diethylamino)phosphinate	C#CCOP(=O)(N(CC)CC)N(CC)CC	DEHSPEZTBSYMPL-UHFFFAOYSA-N	1.9	(*11*)
pentamethyl(prop-2-ynyl)phophoric triamide	C#CCN(C)P(=O)(N(C)C)N(C)C	DOYODMYEMDHHCE-UHFFFAOYSA-N	1.9	(*7*)
ethynyl(trimethyl)silane	C#C[Si](C)(C)C	CWMFRHBXRUITQE-UHFFFAOYSA-N	1.9	(*7*)
n,n,n',n'-tetramethyl-n"-benzyl-n' '-prop-2-ynylphosphoric triamide	C#CCN(Cc1ccccc1)P(=O)(N(C)C)N(C)C	HXRJCRXYCLFNPC-UHFFFAOYSA-N	1.9	(*7*)
ethoxyacetylene	C#COCC	WMYNMYVRWWCRPS-UHFFFAOYSA-N	1.9	(*12*)
1-heptyne	C#CCCCCC	YVXHZKKCZYLQOP-UHFFFAOYSA-N	1.9	(*7*)(*12*)(*9*)
triethyl(ethynyl)silane	C#C[Si](CC)(CC)CC	FWSPXZXVNVQHIF-UHFFFAOYSA-N	1.9,2.0	(*7*)(*12*)
prop-2-ynyl bis(dibutylamido)phosphinate	C#CCOP(=O)(N(CCCC)CCCC)N(CCCC)CCCC	UIZVATMSLGDSAW-UHFFFAOYSA-N	2.0	(*7*)
prop-2-ynyl bis(dimethylamido)phosphinate	C#CCOP(=O)(N(C)C)N(C)C	MFXVLTAAMOAZMS-UHFFFAOYSA-N	2.0	(*7*)

Common Name	**Canonical Smiles**	**InChIKey**	α	**References**
prop-2-ynyl bis(dimethylamino)phosphinate	C#CCOP(=O)(N(C)C)N(C)C	MFXVLTAAMOAZMS-UHFFFAOYSA-N	2.0	(*11*)
o-prop-2-ynyl bis(dimethylamino)thiophosphinate	C#CCOP(=S)(N(C)C)N(C)C	HDWKOGROOOQOOX-UHFFFAOYSA-N	2.0	(*11*)
prop-2-ynyl bis(dibutylamino)phosphinate	C#CCOP(=O)(N(CCCC)CCCC)N(CCCC)CCCC	UIZVATMSLGDSAW-UHFFFAOYSA-N	2.0	(*11*)
o-prop-2-ynyl bis(dimethylamido)thiophosphinate	C#CCO[PH](S)(N(C)C)N(C)C	PQWIYMXWMUTCOW-UHFFFAOYSA-N	2.0	(*7*)
prop-2-ynyl bis(dimethylamido)phosphinate	C#CCP(=O)(N(C)C)N(C)C	JGUWOBGMRMMXJZ-UHFFFAOYSA-N	2.0	(*7*)
3-chloro-3-methyl-1-butyne	C#CC(C)(C)Cl	QSILYWCNPOLKPN-UHFFFAOYSA-N	2.0	(*7*)(*7*)
(ethylsulfanyl)acetylene	C#CSCC	SUFGUGHOVHXSII-UHFFFAOYSA-N	2.1	(*12*)
1-[aziridin-1-yl(prop-2-ynoxy)phosphoryl]aziridine	C#CCOP(=O)(N1CC1)N1CC1	DMGBLQXOZQWUAR-UHFFFAOYSA-N	2.1	(*11*)
prop-2-ynyl bis(morpholino)phosphinate	C#CCOP(=O)(N1CCOCC1)N1CCOCC1	ZWZFGONTTYIELP-UHFFFAOYSA-N	2.1	(*11*)
s-prop-2-ynyl bis(dimethylamido)thiophosphinate	C#CCOP(=S)(N(C)C)N(C)C	HDWKOGROOOQOOX-UHFFFAOYSA-N	2.1	(*11*)
1-bromo-4-ethynylbenzene	C#Cc1ccc(Br)cc1	LTLVZQZDXQWLHU-UHFFFAOYSA-N	2.1	(*12*)
s-prop-2-ynyl bis(dimethylamido)thiophosphinate	C#CCSP(=S)(N(C)C)N(C)C	KPLPKFHCOXVGLK-UHFFFAOYSA-N	2.1	(*7*)
1-phenyl-2-propyn-1-one	C#CC(=O)c1ccccc1	JITPLZPWKYUTDM-UHFFFAOYSA-N	2.1	(*7*)
1-ethynyl-4-nitrobenzene	C#Cc1ccc([N+](=O)[O-])cc1	GAZZTEJDUGESGQ-UHFFFAOYSA-N	2.1	(*12*)
s-prop-2-ynyl bis(dimethylamino)thiophosphinate	C#CCSP(=O)(N(C)C)N(C)C	JEFWAOURROPQAD-UHFFFAOYSA-N	2.1	(*11*)
di-morpholin-4-yl-phosphinic acid prop-2-ynyl ester	CC#CP(=O)(N1CCOCC1)N1CCOCC1	ZWZFGONTTYIELP-UHFFFAOYSA-N	2.1	(*11*)
ethynylbenzene	C#Cc1ccccc1	UEXCJVNBTNXOEH-UHFFFAOYSA-N	2.1,2.0,1.6	(*7*)(*12*)(*8*)
3-bromo-1-propyne	C#CCBr	YORCIIVHUBAYBQ-UHFFFAOYSA-N	2.1	(*7*)(*12*)
3-chloro-1-propyne	C#CCCl	LJZPPWWHKPGCHS-UHFFFAOYSA-N	2.1	(*7*)(*12*)
diethyl prop-2-ynyl phosphate	C#CCOP(=O)(OCC)OCC	BURXZHCIEDSVSW-UHFFFAOYSA-N	2.2	(*7*)
diethyl prop-2-ynyl phosphate	C#CCP(=O)(OCC)OCC	KMUZWGCQPPCIKM-UHFFFAOYSA-N	2.2	(*7*)
ethyl propiolate	C#CC(=O)OCC	FMVJYQGSRWVMQV-UHFFFAOYSA-N	2.3	(*12*)
3-butyn-2-one	C#CC(C)=O	XRGPFNGLRSIPSA-UHFFFAOYSA-N	2.3	(*12*)
3,3,3-trifluoro-1-propyne	C#CC(F)(F)F	PRDFNJUWGIQQBW-UHFFFAOYSA-N	2.5	(*12*)
propiolonitrile	C#CC#N	LNDJVIYUJOJFSO-UHFFFAOYSA-N	2.8	(*12*)

2.2 NH HYDROGEN

2.2.1 AMMONIA

Common Name	Canonical Smiles	InChIKey	α	References
ammonia	N	QGZKDVFQNNGYKY-UHFFFAOYSA-N	3.1	(7)

2.2.2 NITROAMINE

Common Name	Canonical Smiles	InChIKey	α	References
n-nitrocyclohexanamine	O=[N+]([O-])NC1CCCCC1	NHEUXRXASLPKGO-UHFFFAOYSA-N	3.6	(7)
n-nitro-1-butanamine	CCCCN[N+](=O)[O-]	FCLOSAGZCUDMFV-UHFFFAOYSA-N	3.7	(7)
n-nitro-1-propanamine	CCCN[N+](=O)[O-]	MCROFHCOHPROAE-UHFFFAOYSA-N	3.7	(7)
n-nitromethanamine	CN[N+](=O)[O-]	ARCZSDSOONGBRX-UHFFFAOYSA-N	3.8	(7)
3-(nitroamino)propanenitrile	N#CCCN[N+](=O)[O-]	BUFUGXVDLHMFEZ-UHFFFAOYSA-N	4.4	(7)
n,3,3,3-tetranitropropylamine	O=[N+]([O-])NCCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	VLFTYFLZHORIBC-UHFFFAOYSA-N	4.5	(7)

2.2.3 HYDROXYLAMINE N-H

Common Name	Canonical Smiles	InChIKey	α	References
n-(benzyloxy)-1-phenylmethanamine	c1ccc(CNOCc2ccccc2)cc1	WUUIYHZKEXDJKH-UHFFFAOYSA-N	2.9	(7)

2.2.4 ANILINE

Common Name	Canonical Smiles	InChIKey	α	References
n-methylaniline	CNc1ccccc1	AFBPFSWMIHJQDM-UHFFFAOYSA-N	2.1	(*7*)
aniline	Nc1ccccc1	PAYRUJLWNCNPSJ-UHFFFAOYSA-N	2.4	(*7*)(*10*)(*9*)
1-naphthalenamine	Nc1cccc2ccccc12	RUFPHBVGCFYCNW-UHFFFAOYSA-N	2.6	(*7*)
4-bromoaniline	Nc1ccc(Br)cc1	WDFQBORIUYODSI-UHFFFAOYSA-N	2.6	(*7*)
n-phenylaniline	c1ccc(Nc2ccccc2)cc1	DMBHHRLKUKUOEG-UHFFFAOYSA-N	2.7	(*7*)(*9*)
2-naphthalenamine	Nc1ccc2ccccc2c1	JBIJLHTVPXGSAM-UHFFFAOYSA-N	2.8	(*7*)
1,2,3,4-tetrahydroquinoline	c1ccc2c(c1)CCCN2	LBUJPTNKIBCYBY-UHFFFAOYSA-N	2.8	(*10*)
2-nitroaniline	Nc1ccccc1[N+](=O)[O-]	DPJCXCZTLWNFOH-UHFFFAOYSA-N	2.9	(*7*)
n-methyl-4-nitroaniline	CNc1ccc([N+](=O)[O-])cc1	XIFJZJPMHNUGRA-UHFFFAOYSA-N	2.9	(*10*)
3-nitroaniline	Nc1cccc([N+](=O)[O-])c1	XJCVRTZCHMZPBD-UHFFFAOYSA-N	3.0	(*7*)
4-nitroaniline	Nc1ccc([N+](=O)[O-])cc1	TYMLOMAKGOJONV-UHFFFAOYSA-N	3.1	(*7*)
5-nitroindoline	O=[N+]([O-])c1ccc2c(c1)CCN2	WJQWYAJTPPYORB-UHFFFAOYSA-N	3.1	(*10*)
2-chloro-4-nitroaniline	Nc1ccc([N+](=O)[O-])cc1Cl	LOCWBQIWHWIRGN-UHFFFAOYSA-N	3.2	(*7*)
4-chloro-2-nitroaniline	Nc1ccc(Cl)cc1[N+](=O)[O-]	PBGKNXWGYQPUJK-UHFFFAOYSA-N	3.2	(*7*)

2.2.5 ANILINE LIKE

Common Name	Canonical Smiles	InChIKey	α	References
2(1h)-pyrimidinimine	Nc1ncccn1	LJXQPZWIHJMPQQ-UHFFFAOYSA-N	2.5	(*7*)
2-pyridinamine	Nc1ccccn1	ICSNLGPSRYBMBD-UHFFFAOYSA-N	2.7	(*7*)
3-aminopyridine	Nc1cccnc1	CUYKNJBYIJFRCU-UHFFFAOYSA-N	2.8	(*7*)
10,11-dihydro-5h-dibenzo[b,f]azepine	c1ccc2c(c1)CCc1ccccc1N2	ZSMRRZONCYIFNB-UHFFFAOYSA-N	2.8	(*10*)
5-pyrimidinamine	Nc1cncnc1	FVLAYJRLBLHIPV-UHFFFAOYSA-N	2.9	(*7*)
4-aminopyrimidine	Nc1ccncn1	OYRRZWATULMEPF-UHFFFAOYSA-N	2.9	(*7*)
4(1h)-pyridinimine	Nc1ccncc1	NUKYPUAOHBNCPY-UHFFFAOYSA-N	3.0	(*7*)
1,3-benzothiazol-2-amine	Nc1nc2ccccc2s1	UHGULLIUJBCTEF-UHFFFAOYSA-N	3.1	(*10*)

2.2.6 AMIDE

Common Name	Canonical Smiles	InChIKey	α	References
n-[4-(diethylamino)phenyl]acetamide	CCN(CC)c1ccc(NC(C)=O)cc1	MBLHLTGHXCTWAO-UHFFFAOYSA-N	2.7	(*10*)
n-hexylheptanamide	CCCCCCNC(=O)CCCCCC	CYWUZSYXTCCCRG-UHFFFAOYSA-N	2.8	(*10*)
methylimidoformic acid	CNC=O	ATHHXGZTWNVVOU-UHFFFAOYSA-N	2.9	(*8*)
n,2,2-trimethylpropanamide	CNC(=O)C(C)(C)C	QMKKJBRRKIKWFK-UHFFFAOYSA-N	2.9	(*10*)
(1z)-n-methylethanimidic acid	CNC(C)=O	OHLUUHNLEMFGTQ-UHFFFAOYSA-N	2.9	(*7*)(*10*)(*9*)
1-oxa-2-azaspiro[4,5]decan-3-one	O=C1CC2(CCCCC2)ON1	MKGAYPNWSNNENI-UHFFFAOYSA-N	3.1	(*10*)
(1e)-n-phenylethanimidic acid	CC(=O)Nc1ccccc1	FZERHIULMFGESH-UHFFFAOYSA-N	3.3	(*10*)
2,2,2-trifluoroacetamide	NC(=O)C(F)(F)F	NRKYWOKHZRQRJR-UHFFFAOYSA-N	3.4	(*10*)
2,2,2-trifluoro-n-phenylacetamide	O=C(Nc1ccccc1)C(F)(F)F	SAPQIENQEZURNZ-UHFFFAOYSA-N	3.9	(*8*)
n-(3-chloro-4-nitrophenyl)acetamide	CC(=O)Nc1ccc([N+](=O)[O-])c(Cl)c1	KUAYZLXOOIEGDN-UHFFFAOYSA-N	4.2	(*10*)
n-[4-nitro-3-(trifluoromethyl)phenyl]acetamide	CC(=O)Nc1ccc([N+](=O)[O-])c(C(F)(F)F)c1	MIHJCLQINRFOLX-UHFFFAOYSA-N	4.2	(*10*)

2.2.7 IMIDE

Common Name	Canonical Smiles	InChIKey	α	References
2-ethyl-2-methylsuccinimide	CC[C@]1(C)CC(=O)NC1=O	HAPOVYFOVVWLRS-SSDOTTSWSA-N	3.4	(*13*)
5-hydroxy-3,4-dihydro-2h-pyrrol-2-one	O=C1CCC(=O)N1	KZNICNPSHKQLFF-UHFFFAOYSA-N	3.4	(*7*)
5-hydroxy-2h-pyrrol-2-one	O=C1C=CC(=O)N1	PEEHTFAAVSWFBL-UHFFFAOYSA-N	3.4	(*7*)(*10*)(*9*)
2-methyl-3-chloromaleimide	CC1=C(Cl)C(=O)NC1=O	PSOSICZGLLPDFA-UHFFFAOYSA-N	3.6	(*13*)
2,3-dichloro-3-methylmaleimide	C[C@]1(Cl)C(=O)NC(=O)[C@@H]1Cl	RPZNJLQPBDKQOG-JLAZNSOCSA-N	4.1	(*13*)
2,2,2-trifluoro-n-(trifluoroacetyl) acetamide	O=C(NC(=O)C(F)(F)F)C(F)(F)F	GMQVFHZSXKJCIV-UHFFFAOYSA-N	4.3	(*10*)
tetrafluorosuccinimide	O=C1NC(=O)C(F)(F)C1(F)F	LHNPDXSWOZFOAO-UHFFFAOYSA-N	5.0	(*13*)

2.2.8 UREA

Common Name	Canonical Smiles	InChIKey	α	References
1-methyl-2-imidazolidinone	CN1CCNC1=O	JTPZTKBRUCILQD-UHFFFAOYSA-N	3.2	(*7*)

2.2.9 CARBAMATE

Common Name	Canonical Smiles	InChIKey	α	References
ethyl hydrogen phenylcarbonimidate	CCOC(=O)Nc1ccccc1	LBKPGNUOUPTQKA-UHFFFAOYSA-N	2.8	(*7*)
oxazolidin-2-one	O=C1NCCO1	IZXIZTKNFFYFOF-UHFFFAOYSA-N	3.4	(*7*)
1,3-thiazolidin-2-one	O=C1NCCS1	SLYRGJDSFOCAAI-UHFFFAOYSA-N	3.6	(*7*)
ethyl nitrocarbamate	CCOC(=O)N[N+](=O)[O-]	YSJKYAHYBFJVKV-UHFFFAOYSA-N	3.9	(*7*)

2.2.10 THIOAMIDE

Common Name	Canonical Smiles	InChIKey	α	References
n-phenylethanethioamide	CC(=S)Nc1ccccc1	MWCGLTCRJJFXKR-UHFFFAOYSA-N	3.4	(*10*)
ethanimidothioic acid	CC(N)=S	YUKQRDCYNOVPGJ-UHFFFAOYSA-N	3.7	(*7*)

2.2.11 THIOCARBAMATE

Common Name	Canonical Smiles	InChIKey	α	References
1,3-oxazolidine-2-thione	S=C1NCCO1	UMURLIQHQSKULR-UHFFFAOYSA-N	4.1	(*7*)
5-methyl-1,3,5-oxadiazole-2(3h)-thione	CN1CNC(=S)O1	KTQKFUVLEWQZRW-UHFFFAOYSA-N	4.4	(*7*)

2.2.12 THIOUREA

Common Name	Canonical Smiles	InChIKey	α	References
1-methyl-2-imidazolidinethione	CN1CCNC1=S	FDDDTDSPQXLQFY-UHFFFAOYSA-N	3.3	(*7*)

2.2.13 DITHIOCARBAMATE

Common Name	Canonical Smiles	InChIKey	α	References
1,3-thiazolidine-2-thione	S=C1NCCS1	WGJCBBASTRWVJL-UHFFFAOYSA-N	3.8	(*7*)

2.2.14 SELENOTHIOCARBAMATE

Common Name	Canonical Smiles	InChIKey	α	References
1-methyl-2-imidazolidineselone	CN1CCNC1=[Se]	QKFKQYNSENDXNW-UHFFFAOYSA-N	3.5	(*7*)
1,3-thiazolidine-2-selone	[Se]=C1NCCS1	IFWSTZNJCOUYHR-UHFFFAOYSA-N	3.9	(*7*)

2.2.15 PYRROLE

Common Name	Canonical Smiles	InChIKey	α	References
1h-pyrrole	c1cc[nH]c1	KAESVJOAVNADME-UHFFFAOYSA-N	3.0,2.8	(*7*)(*10*)(*8*)(*9*)
1h-indole	c1ccc2[nH]ccc2c1	SIKJAQJRHWYJAI-UHFFFAOYSA-N	3.1	(*7*)
9h-carbazole	c1ccc2c(c1)[nH]c1ccccc12	UJOBWOGCFQCDNV-UHFFFAOYSA-N	3.3	(*7*)
5-fluoro-1h-indole	Fc1ccc2[nH]ccc2c1	ODFFPRGJZRXNHZ-UHFFFAOYSA-N	3.3	(*7*)(*9*)
2,3,4,5-tetraiodo-1h-pyrrole	Ic1[nH]c(I)c(I)c1I	VJOVAKSZILJDBB-UHFFFAOYSA-N	3.8	(*7*)
2,3,4,5-tetrabromo-1h-pyrrole	Brc1[nH]c(Br)c(Br)c1Br	MIIWISWSCMVZHG-UHFFFAOYSA-N	4.2	(*7*)
tetrachloropyrrole	Clc1[nH]c(Cl)c(Cl)c1Cl	NBXDXMFYTJNWCS-UHFFFAOYSA-N	4.3	(*7*)

2.2.16 N HETEROCYCLE

Common Name	Canonical Smiles	InChIKey	α	References
3-(1h-imidazol-2-yl)propyl benzoate	O=C(OCCCc1ncc[nH]1)c1ccccc1	HDJGQEDLEYXGCN-UHFFFAOYSA-N	3.2	(*10*)
5-methyl-4-(2-methyl-2-propanyl)-1, 3-thiazol-2(3h)-one	Cc1sc(=O)[nH]c1C(C)(C)C	XSQWEWUZBUNKAO-UHFFFAOYSA-N	3.2,3.7	(*7*)(*7*)(*7*)
3-(1h-imidazol-2-yl)propyl phenyl c arbanoate	O=C(OCCCc1ncc[nH]1)Oc1ccccc1	UQXAGNCUOPPUJH-UHFFFAOYSA-N	3.4	(*14*)
3,4,5-trimethyl-1h-pyrazole	Cc1n[nH]c(C)c1C	HUVAAOZUPLEYBH-UHFFFAOYSA-N	3.4	(*8*)
4-methyl-1h-pyrazole	Cc1cn[nH]c1	RIKMMFOAQPJVMX-UHFFFAOYSA-N	3.5	(*8*)
4-isopropyl-5-methyl-1,3-thiazole-2 (3h)-thione	Cc1sc(=S)[nH]c1C(C)C	ADBSTNAYQBHUDD-UHFFFAOYSA-N	3.6	(*7*)
3-methyl-1h-pyrazole	Cc1ccn[nH]1	XKVUYEYANWFIJX-UHFFFAOYSA-N	3.6	(*8*)
1h-pyrazole	c1cn[nH]c1	WTKZEGDFNFYCGP-UHFFFAOYSA-N	3.6	(*8*)
3,5-dimethyl-1h-pyrazole	Cc1cc(C)[nH]n1	SDXAWLJRERMRKF-UHFFFAOYSA-N	3.6	(*8*)
3-triazolepropylphenyl	c1ccc(CCCc2nc[nH]n2)cc1	ZOUYLAPTOZAWHX-UHFFFAOYSA-N	3.8	(*10*)
5-nitroindole	O=[N+]([O-])c1ccc2[nH]c cc2c1	OZFPSOBLQZPIAV-UHFFFAOYSA-N	3.8	(*4*)
4-bromo-1h-pyrazole	Brc1cn[nH]c1	WVGCPEDBFHEHEZ-UHFFFAOYSA-N	3.9	(*8*)
4-methyl-1,3-thiazole-2(3h)-thione	Cc1csc(=S)[nH]1	NLHAIPFBNQZTMY-UHFFFAOYSA-N	3.9	(*7*)
4-bromo-3,5-dimethyl-1h-pyrazole	Cc1n[nH]c(C)c1Br	RISOHYOEPYWKOB-UHFFFAOYSA-N	3.9	(*8*)
1,4,5-trimethyl-1,3-dihydro-2h-imid azole-2-thione	Cc1[nH]c(=S)n(C)c1C	PERWAYOEWJEJNO-UHFFFAOYSA-N	3.9	(*7*)
3-methylthio-1,2,3-triazole	CSc1c[nH]nn1	VEDXNNRTYCLCMP-UHFFFAOYSA-N	3.9	(*10*)
1-methyl-1,3-dihydro-2h-benzimidazo l-2-one	Cn1c(=O)[nH]c2ccccc21	PYEHNKXDXBNHQQ-UHFFFAOYSA-N	3.9	(*7*)
4-ethyl-1,3-thiazole-2(3h)-thione	CCc1csc(=S)[nH]1	FORKADXOPFAOHL-UHFFFAOYSA-N	3.9,4.3	(*7*)(*7*)
5-methyl-1,4,5-thiadiazole-2(3h)-th ione	CN1NCC(=S)S1	PEZNCYJTYWZHOG-UHFFFAOYSA-N	4.0	(*7*)
4,5-dimethyl-1,3-oxazol-2(3h)-one	Cc1[nH]c(=O)oc1C	XFHVEEHRWSWVGA-UHFFFAOYSA-N	4.0	(*7*)
1h-benzimidazole-2-thiol	S=c1[nH]c2ccccc2[nH]1	YHMYGUUIMTVXNW-UHFFFAOYSA-N	4.0	(*7*)
1,3-thiazole-2(3h)-thione	S=c1[nH]ccs1	OCVLSHAVSIYKLI-UHFFFAOYSA-N	4.0,4.3	(*7*)(*7*)
4-methyl-1,3-thiazol-2(3h)-one	Cc1csc(=O)[nH]1	ZMEVDFFLOPFGCR-UHFFFAOYSA-N	4.1	(*7*)
4-ethyl-5-methyl-1,3-thiazole-2(3h) -thione	CCc1[nH]c(=S)sc1C	MOZAVBNQQPUPNA-UHFFFAOYSA-N	4.2,3.8	(*7*)(*7*)
4-isopropyl-1,3-thiazole-2(3h)-thione	CC(C)c1csc(=S)[nH]1	BACKYMNXXFPCRL-UHFFFAOYSA-N	4.2,3.8	(*7*)(*7*)
1,3-benzothiazol-2(3h)-one	O=c1[nH]c2ccccc2s1	YEDUAINPPJYDJZ-UHFFFAOYSA-N	4.3	(*7*)
4,5-dimethyl-1,3-thiazole-2(3h)-thione	Cc1[nH]c(=S)sc1C	KKHBRTFQIYIHEI-UHFFFAOYSA-N	4.3	(*7*)
4,5-dimethyl-1,3-oxazole-2(3h)-thione	Cc1[nH]c(=S)oc1C	XEJIHKUDPINBCS-UHFFFAOYSA-N	4.3	(*7*)

Common Name	Canonical Smiles	InChIKey	α	References
4-(trifluoromethyl)-1h-1,2,3-triazole	FC(F)(F)c1c[nH]nn1	DIBFBUQGVMZWTM-UHFFFAOYSA-N	4.3	(*10*)
4-phenyl-1,3-thiazole-2(3h)-thione	S=c1[nH]c(-c2ccccc2)cs1	CYCKHTAVNBPQDB-UHFFFAOYSA-N	4.3	(*7*)
4-(2-methyl-2-propanyl)-1,3-thiazole-2(3h)-thione	CC(C)(C)c1csc(=S)[nH]1	LORVDQSPQDOFQN-UHFFFAOYSA-N	4.3,3.8	(*7*)(*7*)
1,3-benzoxazol-2(3h)-one	O=c1[nH]c2ccccc2o1	ASSKVPFEZFQQNQ-UHFFFAOYSA-N	4.4	(*7*)
2,5-dimethyl-1,2-dihydro-3h-1,2,4-triazole-3-thione	Cc1nn(C)c(=S)[nH]1	FPTMVKXIMZNRJX-UHFFFAOYSA-N	4.5	(*7*)
1,3-benzothiazole-2(3h)-thione	S=c1[nH]c2ccccc2s1	YXIWHUQXZSMYRE-UHFFFAOYSA-N	4.5	(*7*)
1,3-benzoxazole-2(3h)-thione	S=c1[nH]c2ccccc2o1	FLFWJIBUZQARMD-UHFFFAOYSA-N	4.6	(*7*)
3-phenyl-1,2,4-thiadiazole-5(2h)-thione	S=c1nc(-c2ccccc2)[nH]s1	NAKQCFRTJSBUPT-UHFFFAOYSA-N	4.9	(*7*)
3-methyl-1,2,4-thiadiazole-5(2h)-thione	Cc1nc(=S)s[nH]1	QPHZWABVAIGWHI-UHFFFAOYSA-N	4.9	(*7*)
5-phenyl-1h-tetrazole	c1ccc(-c2nn[nH]n2)cc1	MARUHZGHZWCEQU-UHFFFAOYSA-N	5.0	(*10*)

2.2.17 HYDROXYALMINE N-H

Common Name	Canonical Smiles	InChIKey	α	References
n,o-dibenzylhydroxylamine	c1ccc(ONOc2ccccc2)cc1	KZXAMWRVRHIWBN-UHFFFAOYSA-N	2.9	(*7*)

2.2.18 SULFONAMIDE

Common Name	Canonical Smiles	InChIKey	α	References
n-benzyl-4-methylbenzenesulfonamide	Cc1ccc(S(=O)(=O)NCc2ccccc2)cc1	WTHKAJZQYNKTCJ-UHFFFAOYSA-N	3.0	(*10*)
n-benzyltoluene-p-sulfonamide	Cc1ccc(S(=O)(=O)Nc2ccccc2)cc1	VLVCWODDMDGANW-UHFFFAOYSA-N	3.0	(*10*)
4-methyl-n-(2-naphthyl)benzenesulfonamide	Cc1ccc(S(=O)(=O)Nc2ccc3ccccc3c2)cc1	HEXCXGXJELSYJW-UHFFFAOYSA-N	3.2	(*10*)
4-methylbenzenesulfonamide	Cc1ccc(S(N)(=O)=O)cc1	LMYRWZFENFIFIT-UHFFFAOYSA-N	3.2	(*10*)

2.3 OH HYDROGEN

2.3.1 WATER

Common Name	Canonical Smiles	InChIKey	α	References
water	O	XLYOFNOQVPJJNP-UHFFFAOYSA-N	2.8	(*7*)(*9*)

2.3.2 ALCOHOL

Common Name	Canonical Smiles	InChIKey	α	References
3-isopropyl-2,2,4,4-tetramethyl-3-pentanol	CC(C)C(O)(C(C)(C)C)C(C)(C)C	DXYPGMZJNUIZMU-UHFFFAOYSA-N	2.2	(*7*)
3-ethyl-2,4-dimethyl-3-pentanol	CCC(O)(C(C)C)C(C)C	PZPYIRQFCOFLGJ-UHFFFAOYSA-N	2.4	(*7*)(*10*)
butan-2-ol	CC[C@@H](C)O	BTANRVKWQNVYAZ-SCSAIBSYSA-N	2.5	(*8*)
2,2,4,4-tetramethyl-3-pentanol	CC(C)(C)C(O)C(C)(C)C	WFJSIIHYYLHRHB-UHFFFAOYSA-N	2.5	(*7*)
cholesterol	CC(C)CCCC(C)(C)[C@@H]1CC[C@H]2[C@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C	CSDUKRUFTFEFBO-PGNZUDIJSA-N	2.6	(*15*)
2-methyl-1-propanol	CC(C)CO	ZXEKIIBDNHEJCQ-UHFFFAOYSA-N	2.6	(*7*)
(3beta,20r)-cholest-5-en-3-ol	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C	HVYWMOMLDIMFJA-DPAQBDIFSA-N	2.6	(*15*)
2-methyl-2-butanol	CCC(C)(C)O	MSXVEPNJUHWQHW-UHFFFAOYSA-N	2.6	(*7*)
cyclohexanol	OC1CCCCC1	HPXRVTGHNJAIIH-UHFFFAOYSA-N	2.6	(*15*)(*16*)
1-propanol	CCCO	BDERNNFJNOPAEC-UHFFFAOYSA-N	2.6	(*10*)(*8*)(*16*)
2-propanol	CC(C)O	KFZMGEQAYNKOFK-UHFFFAOYSA-N	2.6,2.7	(*7*)(*15*)(*10*)(*8*)(*9*)
2,2-dimethyl-1-propanol	CC(C)(C)CO	KPSSIOMAKSHJJG-UHFFFAOYSA-N	2.7	(*7*)
1-hexanol	CCCCCCO	ZSIAUFGUXNUGDI-UHFFFAOYSA-N	2.7	(*10*)
butan-1-ol	CCCCO	LRHPLDYGYMQRHN-UHFFFAOYSA-N	2.7	(*7*)(*15*)
2-methyl-2-propanol	CC(C)(C)O	DKGAVHZHDRPRBM-UHFFFAOYSA-N	2.7,2.6	(*7*)(*10*)(*8*)(*9*)(*16*)
ethanol	CCO	LFQSCWFLJHTTHZ-UHFFFAOYSA-N	2.7,2.6	(*7*)(*15*)(*10*)(*8*)(*9*)
2-chloroethanol	OCCCl	SZIFAVKTNFCBPC-UHFFFAOYSA-N	2.9	(*15*)
methanol	CO	OKKJLVBELUTLKV-UHFFFAOYSA-N	2.9,2.8,2.7	(*7*)(*15*)(*10*)(*8*)(*9*)
phenylmethanol	OCc1ccccc1	WVDDGKGOMKODPV-UHFFFAOYSA-N	3.0	(*7*)
1,1,1-trichloro-2-methyl-2-propanol	CC(C)(O)C(Cl)(Cl)Cl	OSASVXMJTNOKOY-UHFFFAOYSA-N	3.0	(*7*)
2-fluoroethanol	OCCF	GGDYAKVUZMZKRV-UHFFFAOYSA-N	3.0	(*7*)(*9*)
2,2,2-tribromoethanol	OCC(Br)(Br)Br	YFDSDPIBEUFTMI-UHFFFAOYSA-N	3.3	(*7*)
(pentafluorophenyl)methanol	OCc1c(F)c(F)c(F)c(F)c1F	PGJYYCIOYBZTPU-UHFFFAOYSA-N	3.3	(*7*)

Common Name	**Canonical Smiles**	**InChIKey**	α	**References**
1,1,1-trifluoro-2-methyl-2-propanol	CC(C)(O)C(F)(F)F	OCGWWLDZAFOHGD-UHFFFAOYSA-N	3.3	(*7*)
2,2,2-trichloroethanol	OCC(Cl)(Cl)Cl	KPWDGTGXUYRARH-UHFFFAOYSA-N	3.4,3.3,3.6	(*7*)(*15*)(*8*)
2,2,3,3-tetrafluoro-1-propanol	OCC(F)(F)C(F)F	NBUKAOOFKZFCGD-UHFFFAOYSA-N	3.5	(*7*)
2,2,2-trifluoroethanol	OCC(F)(F)F	RHQDFWAXVIIEBN-UHFFFAOYSA-N	3.7,3.9	(*7*)(*8*)(*9*)
1,1,1,3,3,3-hexachloro-2-propanol	OC(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl	QHSCXYZVJCEABQ-UHFFFAOYSA-N	4.0	(*7*)
1,1,1,3,3,3-hexafluoro-2-methyl-2-propanol	CC(O)(C(F)(F)F)C(F)(F)F	FQDXJYBXPOMIBX-UHFFFAOYSA-N	4.0	(*7*)
1,1,1-trichloro-3,3,3-trifluoro-2-(trifluoromethyl)-2-propanol	OC(C(F)(F)F)(C(F)(F)F)C(Cl)(Cl)Cl	AMCTWDASUQVRCQ-UHFFFAOYSA-N	4.4	(*7*)
1,1,1,3,3,3-hexafluoro-2-propanol	OC(C(F)(F)F)C(F)(F)F	BYEAHWXPCBROCE-UHFFFAOYSA-N	4.5,4.6	(*7*)(*10*)(*8*)(*9*)
1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)-2-propanol	OC(C(F)(F)F)(C(F)(F)F)C(F)(F)F	XZNOAVNRSFURIR-UHFFFAOYSA-N	4.9	(*7*)(*9*)

2.3.3 PHENOL

Common Name	Canonical Smiles	InChIKey	α	References
2-methoxyphenol	COc1ccccc1O	LHGVFZTZFXWLCP-UHFFFAOYSA-N	2.4	(*7*)
2,6-dichlorophenol	Oc1c(Cl)cccc1Cl	HOLHYSJJBXSLMV-UHFFFAOYSA-N	2.7	(*7*)(*10*)
2,6-diisopropylphenol	CC(C)c1cccc(C(C)C)c1O	OLBCVFGFOZPWHH-UHFFFAOYSA-N	2.8	(*15*)
(o- 2 h)phenol	Oc1ccccc1	ISWSIDIOOBJBQZ-UHFFFAOYSA-N	2.8	(*7*)
2-methyl-6-(2-methyl-2-propanyl)phenol	Cc1cccc(C(C)(C)C)c1O	BKZXZGWHTRCFPX-UHFFFAOYSA-N	2.9	(*7*)
2,4,6-trimethylphenol	Cc1cc(C)c(O)c(C)c1	BPRYUXCVCCNUFE-UHFFFAOYSA-N	2.9,3.0	(*7*)(*15*)
2,6-dimethylphenol	Cc1cccc(C)c1O	NXXYKOUNUYWIHA-UHFFFAOYSA-N	3.0	(*7*)
4-bromo-2,6-dimethylphenol	Cc1cc(Br)cc(C)c1O	ZLVFYUORUHNMBO-UHFFFAOYSA-N	3.3	(*7*)
pentabromophenol	Oc1c(Br)c(Br)c(Br)c(Br)c1Br	SVHOVVJFOWGYJO-UHFFFAOYSA-N	3.4	(*7*)
2-(2-methyl-2-propanyl)phenol	CC(C)(C)c1ccccc1O	WJQOZHYUIDYNHM-UHFFFAOYSA-N	3.4,3.5	(*7*)(*15*)
2,3,5-trimethylphenol	Cc1cc(C)c(C)c(O)c1	OGRAOKJKVGDSFR-UHFFFAOYSA-N	3.5	(*7*)
2,3-dimethylphenol	Cc1cccc(O)c1C	QWBBPBRQALCEIZ-UHFFFAOYSA-N	3.5	(*7*)
3-(dimethylamino)phenol	CN(C)c1cccc(O)c1	MESJRHHDBDCQTH-UHFFFAOYSA-N	3.5	(*7*)
2,4-dimethylphenol	Cc1ccc(O)c(C)c1	KUFFULVDNCHOFZ-UHFFFAOYSA-N	3.5	(*7*)
o-cresol	Cc1ccccc1O	QWVGKYWNOKOFNN-UHFFFAOYSA-N	3.5,3.6	(*7*)(*15*)
2,4-bis(2-methyl-2-propanyl)phenol	CC(C)(C)c1ccc(O)c(C(C)(C)C)c1	ICKWICRCANNIBI-UHFFFAOYSA-N	3.6	(*7*)
4-octylphenol	CCCCCCCCc1ccc(O)cc1	NTDQQZYCCIDJRK-UHFFFAOYSA-N	3.6	(*7*)
2-isopropylphenol	CC(C)c1ccccc1O	CRBJBYGJVIBWIY-UHFFFAOYSA-N	3.6	(*7*)
4-(2-methyl-2-propanyl)phenol	CC(C)(C)c1ccc(O)cc1	QHPQWRBYOIRBIT-UHFFFAOYSA-N	3.6	(*7*)
4-ethylphenol	CCc1ccc(O)cc1	HXDOZKJGKXYMEW-UHFFFAOYSA-N	3.6	(*7*)
3-ethylphenol	CCc1cccc(O)c1	HMNKTRSOROOSPP-UHFFFAOYSA-N	3.6	(*7*)
3,4,5-trimethylphenol	Cc1cc(O)cc(C)c1C	FDQQNNZKEJIHMS-UHFFFAOYSA-N	3.6	(*7*)
3,4-dimethylphenol	Cc1ccc(O)cc1C	YCOXTKKNXUZSKD-UHFFFAOYSA-N	3.6	(*7*)
5-methyl-2-(2-methyl-2-propanyl)phenol	Cc1ccc(C(C)(C)C)c(O)c1	XOUQAVYLRNOXDO-UHFFFAOYSA-N	3.6	(*7*)
pentachlorophenol	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	IZUPBVBPLAPZRR-UHFFFAOYSA-N	3.6	(*7*)
4-propylphenol	CCCc1ccc(O)cc1	KLSLBUSXWBJMEC-UHFFFAOYSA-N	3.6	(*7*)
4-isopropylphenol	CC(C)c1ccc(O)cc1	YQUQWHNMBPIWGK-UHFFFAOYSA-N	3.6	(*7*)(*7*)
2,5-dimethylphenol	Cc1ccc(C)c(O)c1	NKTOLZVEWDHZMU-UHFFFAOYSA-N	3.6	(*7*)(*7*)
4-methoxyphenol	COc1ccc(O)cc1	NWVVVBRKAWDGAB-UHFFFAOYSA-N	3.7	(*7*)
4-methyl-2-(2-methyl-2-propanyl)phenol	Cc1ccc(O)c(C(C)(C)C)c1	IKEHOXWJQXIQAG-UHFFFAOYSA-N	3.7	(*7*)
4-sec-butylphenol	CC[C@H](C)c1ccc(O)cc1	ZUTYZAFDFLLILI-QMMMGPOBSA-N	3.7	(*7*)

Common Name	**Canonical Smiles**	**InChIKey**	α	**References**
3-isopropylphenol	CC(C)c1cccc(O)c1	VLJSLTNSFSOYQR-UHFFFAOYSA-N	3.7	(*10*)
3,5-dimethylphenol	Cc1cc(C)cc(O)c1	TUAMRELNJMMDMT-UHFFFAOYSA-N	3.7,3.6	(*7*)(*15*)
m-cresol	Cc1cccc(O)c1	RLSSMJSEOOYNOY-UHFFFAOYSA-N	3.7,3.6	(*7*)(*15*)
p-cresol	Cc1ccc(O)cc1	IWDCLRJOBJJRNH-UHFFFAOYSA-N	3.7	(*7*)(*15*)
3-methoxyphenol	COc1cccc(O)c1	ASHGTJPOSUFTGB-UHFFFAOYSA-N	3.8	(*7*)
1-naphthol	Oc1cccc2ccccc12	KJCVRFUGPWSIIH-UHFFFAOYSA-N	3.8	(*7*)
4-biphenylol	Oc1ccc(-c2ccccc2)cc1	YXVFYQXJAXKLAK-UHFFFAOYSA-N	3.8	(*7*)
phenol	Oc1ccccc1	ISWSIDIOOBJBQZ-UHFFFAOYSA-N	3.8,3.9	(*7*)(*15*)(*8*)(*9*)
2-naphthol	Oc1ccc2ccccc2c1	JWAZRIHNYRIHIV-UHFFFAOYSA-N	3.9	(*7*)
4-fluorophenol	Oc1ccc(F)cc1	RHMPLDJJXGPMEX-UHFFFAOYSA-N	3.9,4.2	(*7*)(*15*)(*8*)(*9*)
2-chlorophenol	Oc1ccccc1Cl	ISPYQTSUDJAMAB-UHFFFAOYSA-N	4.0	(*7*)
3-fluorophenol	Oc1cccc(F)c1	SJTBRFHBXDZMPS-UHFFFAOYSA-N	4.1	(*7*)
4-iodophenol	Oc1ccc(I)cc1	VSMDINRNYYEDRN-UHFFFAOYSA-N	4.1	(*7*)
4-bromophenol	Oc1ccc(Br)cc1	GZFGOTFRPZRKDS-UHFFFAOYSA-N	4.1	(*7*)
2,3,4,5,6,7,8-heptafluoro-1-naphthol	Oc1c(F)c(F)c(F)c2c(F)c(F)c(F)c(F)c12	ODAJDDMWMREWGL-UHFFFAOYSA-N	4.1	(*7*)
4-chlorophenol	Oc1ccc(Cl)cc1	WXNZTHHGJRFXKQ-UHFFFAOYSA-N	4.1,4.2	(*7*)(*8*)(*9*)
3-chlorophenol	Oc1cccc(Cl)c1	HORNXRXVQWOLPJ-UHFFFAOYSA-N	4.2	(*7*)
methyl 3-hydroxybenzoate	COC(=O)c1cccc(O)c1	YKUCHDXIBAQWSF-UHFFFAOYSA-N	4.2	(*8*)
2,6-dichloro-4-nitrophenol	O=[N+]([O-])c1cc(Cl)c(O)c(C l)c1	PXSGFTWBZNPNIC-UHFFFAOYSA-N	4.2	(*7*)
3-bromophenol	Oc1cccc(Br)c1	MNOJRWOWILAHAV-UHFFFAOYSA-N	4.2	(*7*)
4-phenylazophenol	Oc1ccc(cc1)\N=N\c2ccccc2	BEYOBVMPDRKTNR-BUHFOSPRSA-N	4.3	(*17*)
3-(trifluoromethyl)phenol	Oc1cccc(C(F)(F)F)c1	UGEJOEBBMPOJMT-UHFFFAOYSA-N	4.3	(*7*)
4-(trifluoromethyl)phenol	Oc1ccc(C(F)(F)F)cc1	BAYGVMXZJBFEMB-UHFFFAOYSA-N	4.3	(*7*)
1-(4-hydroxyphenyl)ethanone	CC(=O)c1ccc(O)cc1	TXFPEBPIARQUIG-UHFFFAOYSA-N	4.3	(*7*)
3,4-dichlorophenol	Oc1ccc(Cl)c(Cl)c1	WDNBURPWRNALGP-UHFFFAOYSA-N	4.4	(*7*)
salicylonitrile	N#Cc1ccccc1O	CHZCERSEMVWNHL-UHFFFAOYSA-N	4.4	(*7*)
3,5-dichlorophenol	Oc1cc(Cl)cc(Cl)c1	VPOMSPZBQMDLTM-UHFFFAOYSA-N	4.5	(*7*)
3-hydroxybenzonitrile	N#Cc1cccc(O)c1	SGHBRHKBCLLVCI-UHFFFAOYSA-N	4.5	(*7*)
1,3,4,5,6,7,8-heptafluoro-2-naphthol	Oc1c(F)c(F)c2c(F)c(F)c(F)c(F)c2c1F	RWEQEWKAJFTONV-UHFFFAOYSA-N	4.5	(*7*)
pentafluorophenol	Oc1c(F)c(F)c(F)c(F)c1F	XBNGYFFABRKICK-UHFFFAOYSA-N	4.5	(*7*)(*8*)
3-nitrophenol	O=[N+]([O-])c1cccc(O)c1	RTZZCYNQPHTPPL-UHFFFAOYSA-N	4.6	(*7*)
4-hydroxybenzonitrile	N#Cc1ccc(O)cc1	CVNOWLNNPYYEOH-UHFFFAOYSA-N	4.6	(*7*)(*9*)

Common Name	Canonical Smiles	InChIKey	α	References
3,4,5-trichlorophenol	Oc1cc(Cl)c(Cl)c(Cl)c1	GBNHEBQXJVDXSW-UHFFFAOYSA-N	4.7	(*7*)
3,5-bis(trifluoromethyl)phenol	Oc1cc(C(F)(F)F)cc(C(F)(F)F)c1	ODSXJQYJADZFJX-UHFFFAOYSA-N	4.7	(*7*)
4-nitrophenol	O=[N+]([O-])c1ccc(O)cc1	BTJIUGUIPKRLHP-UHFFFAOYSA-N	4.7	(*7*)(*10*)(*9*)
4-nitro-3-(trifluoromethyl)phenol	O=[N+]([O-])c1ccc(O)cc1C(F)(F)F	ZEFMBAFMCSYJOO-UHFFFAOYSA-N	5.3	(*7*)

2.3.4 CARBOXYLIC ACID

Common Name	Canonical Smiles	InChIKey	α	References
hexanoic acid	CCCCCC(=O)O	FUZZWVXGSFPDMH-UHFFFAOYSA-N	3.3	(*7*)
pivalic acid	CC(C)(C)C(=O)O	IUGYQRQAERSCNH-UHFFFAOYSA-N	3.5	(*7*)
acetic acid	CC(=O)O	QTBSBXVTEAMEQO-UHFFFAOYSA-N	3.7,3.6	(*7*)(*10*)(*9*)
benzoic acid	O=C(O)c1ccccc1	WPYMKLBDIGXBTP-UHFFFAOYSA-N	3.8	(*7*)
2-bromobenzoic acid	O=C(O)c1ccccc1Br	XRXMNWGCKISMOH-UHFFFAOYSA-N	4.0	(*7*)
chloroacetic acid	O=C(O)CCl	FOCAUTSVDIKZOP-UHFFFAOYSA-N	4.7,4.4	(*7*)(*9*)
pentafluorobenzoic acid	O=C(O)c1c(F)c(F)c(F)c(F)c1F	YZERDTREOUSUHF-UHFFFAOYSA-N	5.0	(*7*)
dichloroacetic acid	O=C(O)C(Cl)Cl	JXTHNDFMNIQAHM-UHFFFAOYSA-N	5.1,5.0	(*7*)(*10*)(*9*)
trichloroacetic acid	O=C(O)C(Cl)(Cl)Cl	YNJBWRMUSHSURL-UHFFFAOYSA-N	5.2	(*7*)(*9*)
trifluoroacetic acid	O=C(O)C(F)(F)F	DTQVDTLACAAQTR-UHFFFAOYSA-N	5.3	(*7*)(*9*)

2.3.5 CYANIC ACID

Common Name	Canonical Smiles	InChIKey	α	References
cyanic acid	N#CO	XLJMAIOERFSOGZ-UHFFFAOYSA-N	3.6	(*7*)

2.3.6 HYDROXYLAMINE O-H

Common Name	Canonical Smiles	InChIKey	α	References
4a-phenyloctahydronaphthalen-2-one oxime	O/N=C1/CC[C@]2(c3ccccc3)CCCC[C@H]2C1	HSQXKKSEAOWACG-GEHXZAHHSA-N	3.0	(*10*)
(e)-2,2-dimethyl hexan-1-phenyl hydroxylamine	CCCCCC(C)(C)/C(=N\O)c1ccccc1	SMBLCBJIVZBEPF-PEZBUJJGSA-N	3.1	(*10*)
n-benzyl-n-hydroxy-1-phenylmethanamine	ON(Cc1ccccc1)Cc1ccccc1	GXELTROTKVKZBQ-UHFFFAOYSA-N	3.2	(*7*)

2.3.7 PEROXY ACID

Common Name	Canonical Smiles	InChIKey	α	References
4-(2-methyl-2-propanyl)benzenecarboperoxoic acid	CC(C)(C)c1ccc(C(=O)OO)cc1	TZAJCDOWOPBMKD-UHFFFAOYSA-N	2.6	(*7*)
3-chlorobenzenecarboperoxoic acid	O=C(OO)c1cccc(Cl)c1	NHQDETIJWKXCTC-UHFFFAOYSA-N	2.9	(*7*)
4-chlorobenzenecarboperoxoic acid	O=C(OO)c1ccc(Cl)cc1	STABAPSYCQFWOK-UHFFFAOYSA-N	2.9	(*7*)

2.3.8 SILANOL

Common Name	Canonical Smiles	InChIKey	α	References
trimethylsilanol	C[Si](C)(C)O	AAPLIUHOKVUFCC-UHFFFAOYSA-N	3.0	(*7*)

2.4 SH HYDROGEN

2.4.1 THIOL

Common Name	Canonical Smiles	InChIKey	α	References
1-butanethiol	CCCCS	WQAQPCDUOCURKW-UHFFFAOYSA-N	1.3	(*7*)
2-propanethiol	CC(C)S	KJRCEJOSASVSRA-UHFFFAOYSA-N	1.3,1.4	(*7*)(*8*)
2-methyl-2-propanethiol	CC(C)(C)S	WMXCDAVJEZZYLT-UHFFFAOYSA-N	1.3,1.5	(*7*)(*8*)
ethanethiol	CCS	DNJIEGIFACGWOD-UHFFFAOYSA-N	1.4	(*8*)
1-propanethiol	CCCS	SUVIGLJNEAMWEG-UHFFFAOYSA-N	1.4	(*8*)
benzenethiol	Sc1ccccc1	RMVRSNDYEFQCLF-UHFFFAOYSA-N	1.7	(*7*)

2.4.2 THIOCYANIC ACID

Common Name	Canonical Smiles	InChIKey	α	References
thiocyanic acid	N#CS	ZMZDMBWJUHKJPS-UHFFFAOYSA-N	4.4	(*7*)

2.5 σ-HOLES

Common Name	Canonical Smiles	InChIKey	α	References
carbon tetrachloride	ClC(Cl)(Cl)Cl	VZGDMQKNWNREIO-UHFFFAOYSA-N	1.4	
dichloromethane	ClCCl	YMWUJEATGCHHMB-UHFFFAOYSA-N	1.4	
carbon tetrabromide	BrC(Br)(Br)Br	HJUGFYREWKUQJT-UHFFFAOYSA-N	2.1	
perfluorohexyl iodide	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I	BULLJMKUVKYZDJ-UHFFFAOYSA-N	2.2-2.6	(*18*)
iodine	II	PNDPGZBMCMUPRI-UHFFFAOYSA-N	2.8	(*19*)

2.6 CATIONS

2.6.1 Metal

Common Name	Canonical Smiles	InChIKey	α	References
rubidium ion	[Rb+]	NCCSSGKUIKYAJD-UHFFFAOYSA-N	3.5	(*5*)
cesium ion	[Cs+]	NCMHKCKGHRPLCM-UHFFFAOYSA-N	3.5	(*5*)
potassium ion	[K+]	NPYPAHLBTDXSSS-UHFFFAOYSA-N	3.6	(*5*)
sodium ion	[Na+]	FKNQFGJONOIPTF-UHFFFAOYSA-N	4.1	(*5*)
lithium ion	[Li+]	HBBGRARXTFLTSG-UHFFFAOYSA-N	5.0	(*5*)

2.6.2 Protonated Nitrogen

Common Name	Canonical Smiles	InChIKey	α	References
n-methyl imidazolium	C[n+]1cc[nH]c1	MCTWTZJPVLRJOU-UHFFFAOYSA-O	4.7	(*5*)
2-ethylhexyl ammonium	CCCCC(CC)CN	LTHNHFOGQMKPOV-UHFFFAOYSA-O	4.8	(*5*)
triethyl ammonium	CC[NH+](CC)CC	ZMANZCXQSJIPKH-UHFFFAOYSA-O	4.8	(*5*)
bis(4-tert-butylphenyl)iodonium	CC(C)(C)c1ccc([I+]c2ccc(C(C)(C)C)cc2)cc1	DNFSNYQTQMVTOK-UHFFFAOYSA-N	4.9	(*5*)
guanidinium	NC(N)=[NH2+]	ZRALSGWEFCBTJO-UHFFFAOYSA-O	5.0	(*5*)

2.6.3 Quaternary Ammonium

Common Name	Canonical Smiles	InChIKey	α	References
tetra(n-butyl)ammonium	CCCC[N+](CCCC)(CCCC)CCCC	DZLFLBLQUQXARW-UHFFFAOYSA-N	2.7	(*5*)
1-methyl,-3-octyl,imidazolium	CCCCCCCCn1cc[n+](C)c1	WXMVWUBWIHZLMQ-UHFFFAOYSA-N	3.3	(*5*)
N-butyl-4-methyl pyridinium	CCCC[n+]1ccc(C)cc1	NNLHWTTWXYBJBQ-UHFFFAOYSA-N	3.5	(*5*)

3 Experimentally Measured Solute β Parameters

3.1 CARBON

3.1.1 ALKENE

Common Name	Canonical Smiles	InChIKey	β	References
cyclohexene	C1=CCCCC1	HGCIXCUEYOPUTN-UHFFFAOYSA-N	1.2	(*20*)
hexa-1,2-diene	C=C=CCCC	XIAJQOBRHVKGSP-UHFFFAOYSA-N	1.7	(*21*)
styrene	C=Cc1ccccc1	PPBRXRYQALVLMV-UHFFFAOYSA-N	2.5	(*21*)

3.1.2 AROMATIC

Common Name	Canonical Smiles	InChIKey	β	References
toluene	Cc1ccccc1	YXFVVABEGXRONW-UHFFFAOYSA-N	2.1	(*21*)
benzene	c1ccccc1	UHOVQNZJYSORNB-UHFFFAOYSA-N	2.1,2.0	(*21*)(*20*)
furan	c1ccoc1	YLQBMQCUIZJEEH-UHFFFAOYSA-N	2.2,2.1	(*22*)(*21*)
thiophene	c1ccsc1	YTPLMLYBLZKORZ-UHFFFAOYSA-N	2.2	(*21*)
ethyl benzene	CCc1ccccc1	YNQLUTRBYVCPMQ-UHFFFAOYSA-N	2.2	(*21*)
o-xylene	Cc1ccccc1C	CTQNGGLPUBDAKN-UHFFFAOYSA-N	2.3	(*21*)
dodecyl benzene	CCCCCCCCCCCCc1ccccc1	KWKXNDCHNDYVRT-UHFFFAOYSA-N	2.4	(*21*)
m-xylene	Cc1cccc(C)c1	IVSZLXZYQVIEFR-UHFFFAOYSA-N	2.4	(*21*)
p-xylene	Cc1ccc(C)cc1	URLKBWYHVLBVBO-UHFFFAOYSA-N	2.5,2.4	(*21*)(*20*)
2,6-di-tert-butylpyridine	CC(C)(C)c1cccc(C(C)(C)C)n1	UWKQJZCTQGMHKD-UHFFFAOYSA-N	1.9,2.6	(*23*)(*21*)
mesitylene	Cc1cc(C)cc(C)c1	AUHZEENZYGFFBQ-UHFFFAOYSA-N	2.7	(*21*)
1,2,4,5-tetramethylbenzene	Cc1cc(C)c(C)cc1C	SQNZJJAZBFDUTD-UHFFFAOYSA-N	2.7	(*21*)
biphenyl	c1ccc(-c2ccccc2)cc1	ZUOUZKKEUPVFJK-UHFFFAOYSA-N	2.7	(*21*)
pentamethylbenzene	Cc1cc(C)c(C)c(C)c1C	BEZDDPMMPIDMGJ-UHFFFAOYSA-N	2.8	(*21*)
naphthalene	c1ccc2ccccc2c1	UFWIBTONFRDIAS-UHFFFAOYSA-N	2.8,2.5	(*21*)(*20*)
phenanthrene	c1ccc2c(c1)ccc1ccccc12	YNPNZTXNASCQKK-UHFFFAOYSA-N	2.9	(*21*)
hexamethylbenzene	Cc1c(C)c(C)c(C)c(C)c1C	YUWFEBAXEOLKSG-UHFFFAOYSA-N	3.3	(*21*)
1-methylpyrrole	Cn1cccc1	OXHNLMTVIGZXSG-UHFFFAOYSA-N	3.6	(*10*)
1h-pyrrole	c1cc[nH]c1	KAESVJOAVNADME-UHFFFAOYSA-N	4.1,3.4	(*10*)(*20*)

3.1.3 ALKYNE

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
butylacetylene	C#CCCCC	CGHIBGNXEGJPQZ-UHFFFAOYSA-N	2.4,2.6	(*21*)(*20*)
1-heptyne	C#CCCCCC	YVXHZKKCZYLQOP-UHFFFAOYSA-N	2.7	(*21*)
hexylacetylene	C#CCCCCCC	UMIPWJGWASORKV-UHFFFAOYSA-N	2.9	(*21*)

3.2 NITROGEN

3.2.1 AMMONIA

Common Name	Canonical Smiles	InChIKey	β	References
ammonia	N	QGZKDVFQNNGYKY-UHFFFAOYSA-N	6.8	(*20*)

3.2.2 PRIMARY AMINE

Common Name	Canonical Smiles	InChIKey	β	References
2,2,2-trifluoroethanamine	NCC(F)(F)F	KIPSRYDSZQRPEA-UHFFFAOYSA-N	4.3,4.6	(*21*)(*24*)(*20*)
1-(3,5-difluorophenyl)methanamine	NCc1cc(F)cc(F)c1	VJNGGOMRUHYAMC-UHFFFAOYSA-N	5.9	(*23*)
3-aminopropanenitrile	N#CCCN	AGSPXMVUFBBBMO-UHFFFAOYSA-N	5.9,6.2	(*10*)(*24*)
1-(3-fluorophenyl)methanamine	NCc1cccc(F)c1	QVSVMNXRLWSNGS-UHFFFAOYSA-N	6.6	(*23*)
2-propyn-1-amine	C#CCN	JKANAVGODYYCQF-UHFFFAOYSA-N	6.6	(*24*)
cyclopropanamine	NC1CC1	HTJDQJBWANPRPF-UHFFFAOYSA-N	6.9	(*24*)
trioctylamine	CCCCCCCCN(CCCCCCCC)CCCCCCCC	XTAZYLNFDRKIHJ-UHFFFAOYSA-N	7.0	(*21*)
1-phenylmethanamine	NCc1ccccc1	WGQKYBSKWIADBV-UHFFFAOYSA-N	7.2,7.1	(*23*)(*21*)(*24*)
1-(3-methylphenyl)methanamine	Cc1cccc(CN)c1	RGXUCUWVGKLACF-UHFFFAOYSA-N	7.4	(*23*)
2-propen-1-amine	C=CCN	VVJKKWFAADXIJK-UHFFFAOYSA-N	7.4	(*10*)(*24*)
hexylamine	CCCCCCN	BMVXCPBXGZKUPN-UHFFFAOYSA-N	7.7	(*21*)
heptylamine	CCCCCCCN	WJYIASZWHGOTOU-UHFFFAOYSA-N	7.7	(*21*)
decylamine	CCCCCCCCCCN	MHZGKXUYDGKKIU-UHFFFAOYSA-N	7.8	(*21*)
methylamine	CN	BAVYZALUXZFZLV-UHFFFAOYSA-N	7.8	(*20*)
pentylamine	CCCCCN	DPBLXKKOBLCELK-UHFFFAOYSA-N	7.8	(*21*)
1-propanamine	CCCN	WGYKZJWCGVVSQN-UHFFFAOYSA-N	7.8,7.9	(*21*)(*24*)
nonylamine	CCCCCCCCCN	FJDUDHYHRVPMJZ-UHFFFAOYSA-N	7.9	(*21*)
2-phenylethanamine	NCCc1ccccc1	BHHGXPLMPWCGHP-UHFFFAOYSA-N	7.9	(*24*)
ethanamine	CCN	QUSNBJAOOMFDIB-UHFFFAOYSA-N	7.9	(*23*)(*24*)
1-butanamine	CCCCN	HQABUPZFAYXKJW-UHFFFAOYSA-N	7.9,8.0	(*21*)(*24*)
2-methyl-2-propanamine	CC(C)(C)N	YBRBMKDOPFTVDT-UHFFFAOYSA-N	7.9,8.0,8.1	(*23*)(*21*)(*24*)

Common Name	Canonical Smiles	InChIKey	β	References
1-octanamine	CCCCCCCCN	IOQPZZOEVPZRBK-UHFFFAOYSA-N	7.9,8.1	(*21*)(*24*)
1,4-diaminobutane	NCCCCN	KIDHWZJUCRJVML-UHFFFAOYSA-N	8.0	(*24*)
1,6-diaminohexane	NCCCCCCN	NAQMVNRVTILPCV-UHFFFAOYSA-N	8.0	(*24*)
2-propanamine	CC(C)N	JJWLVOIRVHMVIS-UHFFFAOYSA-N	8.0	(*21*)(*24*)
n-hexadecylamine	CCCCCCCCCCCCCCCCN	FJLUATLTXUNBOT-UHFFFAOYSA-N	8.1	(*24*)
2-methoxyethylamine	COCCN	ASUDFOJKTJLAIK-UHFFFAOYSA-N	8.1	(*24*)
3-methoxypropylamine	COCCCN	FAXDZWQIWUSWJH-UHFFFAOYSA-N	8.1	(*24*)
cyclohexanamine	NC1CCCCC1	PAFZNILMFXTMIY-UHFFFAOYSA-N	8.1	(*24*)
octadecylamine	CCCCCCCCCCCCCCCCCCCN	REYJJPSVUYRZGE-UHFFFAOYSA-N	8.1	(*21*)
1-adamantanamine	N[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2	DKNWSYNQZKUICI-CHIWXEEVSA-N	8.2	(*24*)
ethylenediamine	NCCN	PIICEJLVQHRZGT-UHFFFAOYSA-N	8.7	(*24*)
1,3-diaminopropane	NCCCN	XFNJVJPLKCPIBV-UHFFFAOYSA-N	8.9	(*24*)

3.2.3 SECONDARY AMINE

Common Name	Canonical Smiles	InChIKey	β	References
dibenzylamine	c1ccc(CNCc2ccccc2)cc1	BWLUMTFWVZZZND-UHFFFAOYSA-N	6.3	(*21*)
morpholine	C1COCCN1	YNAVUWVOSKDBBP-UHFFFAOYSA-N	7.2	(*21*)(*20*)
di-isopropylamine	CC(C)NC(C)C	UAOMVDZJSHZZME-UHFFFAOYSA-N	7.5	(*21*)
1,2,3,6-tetrahydropyridine	C1=CCNCC1	FTAHXMZRJCZXDL-UHFFFAOYSA-N	7.9	(*23*)
dipentylamine	CCCCCNCCCCC	JACMPVXHEARCBO-UHFFFAOYSA-N	7.9	(*21*)
dibutylamine	CCCCNCCCC	JQVDAXLFBXTEQA-UHFFFAOYSA-N	7.9	(*21*)
dipropylamine	CCCNCCC	WEHWNAOGRSTTBQ-UHFFFAOYSA-N	7.9	(*21*)
diethylamine	CCNCC	HPNMFZURTQLUMO-UHFFFAOYSA-N	7.9,7.8	(*21*)(*21*)
n-methylethylamine	CCNC	LIWAQLJGPBVORC-UHFFFAOYSA-N	8.1	(*23*)
dimethylamine	CNC	ROSDSFDQCJNGOL-UHFFFAOYSA-N	8.1	(*23*)
piperidine	C1CCNCC1	NQRYJNQNLNOLGT-UHFFFAOYSA-N	8.3	(*23*)(*21*)(*20*)
5-methyl-2,3-dihydro-1h-pyrrole	CC1=CCCN1	MUUWQYQRBFVTIB-UHFFFAOYSA-N	8.7	(*23*)
azetidine	C1CNC1	HONIICLYMWZJFZ-UHFFFAOYSA-N	8.8	(*23*)
pyrrolidine	C1CCNC1	RWRDLPDLKQPQOW-UHFFFAOYSA-N	8.8	(*23*)

3.2.4 TERTIARY AMINE

Common Name	Canonical Smiles	InChIKey	β	References
triphenylamine	c1ccc(N(c2ccccc2)c2ccccc2)cc1	ODHXBMXNKOYIBV-UHFFFAOYSA-N	3.6	(*21*)
tribenzylamine	c1ccc(CN(Cc2ccccc2)Cc2ccccc2)cc1	MXHTZQSKTCCMFG-UHFFFAOYSA-N	3.8	(*21*)
1,2,2,6,6-pentamethylpiperidine	CN1C(C)(C)CCCC1(C)C	XULIXFLCVXWHRF-UHFFFAOYSA-N	5.8	(*23*)
hexamethylenetetramine	C1N2CN3CN1CN(C2)C3	VKYKSIONXSXAKP-UHFFFAOYSA-N	6.0	(*23*)
n,n-diallyl-2-propen-1-amine	C=CCN(CC=C)CC=C	VPYJNCGUESNPMV-UHFFFAOYSA-N	6.1	(*21*)
tripropylamine	CCCN(CCC)CCC	YFTHZRPMJXBUME-UHFFFAOYSA-N	6.6	(*21*)
n,n-dimethyl-2-propyn-1-amine	C#CCN(C)C	ILBIXZPOMJFOJP-UHFFFAOYSA-N	6.6	(*23*)
n,n-dimethyl-1-phenylmethanamine	CN(C)Cc1ccccc1	XXBDWLFCJWSEKW-UHFFFAOYSA-N	6.6,6.8	(*23*)(*21*)
tributylamine	CCCCN(CCCC)CCCC	IMFACGCPASFAPR-UHFFFAOYSA-N	6.8	(*21*)
tripentylamine	CCCCCN(CCCCC)CCCCC	OOHAUGDGCWURIT-UHFFFAOYSA-N	6.9	(*21*)
n-methylmorpholine	CN1CCOCC1	SJRJJKPEHAURKC-UHFFFAOYSA-N	6.9	(*21*)
n,n'-dimethylpiperazine	CN1CCN(C)CC1	RXYPXQSKLGGKOL-UHFFFAOYSA-N	7.2	(*23*)
1-(4-nitrobenzyl)piperidine	O=[N+]([O-])c1ccc(CN2CCCCC2)cc1	PAMJENUKCYUKLC-UHFFFAOYSA-N	6.9	(*21*)
n,n-dimethyl-2-propen-1-amine	C=CCN(C)C	GBCKRQRXNXQQPW-UHFFFAOYSA-N	7.3	(*23*)
3-chloroquinuclidine	Cl[C@H]1CN2CCC1CC2	NOLVABYTFMDREN-ZETCQYMHSA-N	7.4	(*23*)
1-methyl-1,2,3,6-tetrahydropyridine	CN1CC=CCC1	AUFIRGPROMANKW-UHFFFAOYSA-N	7.5	(*23*)
triethylamine	CCN(CC)CC	ZMANZCXQSJIPKH-UHFFFAOYSA-N	7.5	(*21*)(*20*)
n-methylpiperidine	CN1CCCCC1	PAMIQIKDUOTOBW-UHFFFAOYSA-N	7.7	(*23*)
trimethylamine	CN(C)C	GETQZCLCWQTVFV-UHFFFAOYSA-N	7.8	(*23*)
cyclohexyldimethylamine	CN(C)C1CCCCC1	SVYKKECYCPFKGB-UHFFFAOYSA-N	7.8	(*21*)
n,n-dimethylethanamine	CCN(C)C	DAZXVJBJRMWXJP-UHFFFAOYSA-N	7.9	(*23*)
1-methylpyrrolidine	CN1CCCC1	AVFZOVWCLRSYKC-UHFFFAOYSA-N	7.9	(*23*)
1,4-diazabicyclo[2.2.2]octane	C1CN2CCN1CC2	IMNIMPAHZVJRPE-UHFFFAOYSA-N	8.9	(*21*)
quinuclidine	C1CN2CCC1CC2	SBYHFKPVCBCYGV-UHFFFAOYSA-N	9.1,8.9	(*23*)(*21*)(*20*)

3.2.5 ANILINE

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
n-phenylaniline	c1ccc(Nc2ccccc2)cc1	DMBHHRLKUKUOEG-UHFFFAOYSA-N	3.2	(*20*)
3-bromoaniline	Nc1cccc(Br)c1	DHYHYLGCQVVLOQ-UHFFFAOYSA-N	3.4	(*21*)
3-iodoaniline	Nc1cccc(I)c1	FFCSRWGYGMRBGD-UHFFFAOYSA-N	3.6	(*21*)
3-chloroaniline	Nc1cccc(Cl)c1	PNPCRKVUWYDDST-UHFFFAOYSA-N	3.6	(*21*)
3-fluoroaniline	Nc1cccc(F)c1	QZVQQUVWFIZUBQ-UHFFFAOYSA-N	3.7	(*21*)
4-iodoaniline	Nc1ccc(I)cc1	VLVCDUSVTXIWGW-UHFFFAOYSA-N	3.8	(*21*)
4-chloroaniline	Nc1ccc(Cl)cc1	QSNSCYSYFYORTR-UHFFFAOYSA-N	4.1	(*21*)
4-bromoaniline	Nc1ccc(Br)cc1	WDFQBORIUYODSI-UHFFFAOYSA-N	4.1	(*21*)(*21*)
n,n-dimethylaniline	CN(C)c1ccccc1	JLTDJTHDQAWBAV-UHFFFAOYSA-N	4.2	(*21*)
4-fluoroaniline	Nc1ccc(F)cc1	KRZCOLNOCZKSDF-UHFFFAOYSA-N	4.3	(*21*)
2-methylaniline	Cc1ccccc1N	RNVCVTLRINQCPJ-UHFFFAOYSA-N	4.5	(*21*)
aniline	Nc1ccccc1	PAYRUJLWNCNPSJ-UHFFFAOYSA-N	4.5,4.3	(*21*)(*20*)
3-methoxyaniline	COc1cccc(N)c1	NCBZRJODKRCREW-UHFFFAOYSA-N	4.7	(*21*)
m-toluidine	Cc1cccc(N)c1	JJYPMNFTHPTTDI-UHFFFAOYSA-N	4.7	(*21*)
p-toluidine	Cc1ccc(N)cc1	RZXMPPFPUUCRFN-UHFFFAOYSA-N	4.9	(*21*)
n,n-diethylaniline	CCN(CC)c1ccccc1	GGSUCNLOZRCGPQ-UHFFFAOYSA-N	4.9	(*21*)
4-methoxyaniline	COc1ccc(N)cc1	BHAAPTBBJKJZER-UHFFFAOYSA-N	5.3	(*21*)

3.2.6 PYRIDINE

Common Name	Canonical Smiles	InChIKey	β	References
pentafluoropyridine	Fc1nc(F)c(F)c(F)c1F	XTGOWLIKIQLYRG-UHFFFAOYSA-N	2.0	(*25*)
2,6-difluoropyridine	Fc1cccc(F)n1	MBTGBRYMJKYYOE-UHFFFAOYSA-N	3.4	(*25*)
3,5-dichloropyridine	Clc1cncc(Cl)c1	WPGHPGAUFIJVJF-UHFFFAOYSA-N	5.0	(*23*)(*25*)
2-fluoropyridine	Fc1ccccn1	MTAODLNXWYIKSO-UHFFFAOYSA-N	5.1,5.2	(*21*)(*25*)
2-bromopyridine	Brc1ccccn1	IMRWILPUOVGIMU-UHFFFAOYSA-N	5.1,5.4	(*21*)(*25*)
nicotinonitrile	N#Cc1cccnc1	GZPHSAQLYPIAIN-UHFFFAOYSA-N	5.2,5.3	(*21*)(*25*)
2-methoxypyridine	COc1ccccn1	IWTFOFMTUOBLHG-UHFFFAOYSA-N	5.3	(*25*)
2-chloropyridine	Clc1ccccn1	OKDGRDCXVWSXDC-UHFFFAOYSA-N	5.3,5.4	(*21*)(*25*)
4-cyanopyridine	N#Cc1ccncc1	GPHQHTOMRSGBNZ-UHFFFAOYSA-N	5.4	(*25*)
2,2'-bipyridine	c1ccc(-c2ccccn2)nc1	ROFVEXUMMXZLPA-UHFFFAOYSA-N	5.6	(*25*)
benzo[h]quinoline	c1ccc2c(c1)ccc1cccnc12	WZJYKHNJTSNBHV-UHFFFAOYSA-N	5.6	(*25*)
2-(2-methyl-2-propanyl)pyridine	CC(C)(C)c1ccccn1	UUIMDJFBHNDZOW-UHFFFAOYSA-N	5.7,6.2	(*21*)(*25*)
3-chloropyridine	Clc1cccnc1	PWRBCZZQRRPXAB-UHFFFAOYSA-N	6.0,5.6	(*23*)(*21*)(*25*)
3-bromopyridine	Brc1cccnc1	NYPYPOZNGOXYSU-UHFFFAOYSA-N	6.0,5.9	(*23*)(*21*)(*25*)
3-iodopyridine	Ic1cccnc1	XDELKSRGBLWMBA-UHFFFAOYSA-N	6.1	(*25*)
3-fluoropyridine	Fc1cccnc1	CELKOWQJPVJKIL-UHFFFAOYSA-N	6.1,6.0	(*23*)(*10*)(*25*)
2-phenylpyridine	c1ccc(-c2ccccn2)cc1	VQGHOUODWALEFC-UHFFFAOYSA-N	6.2	(*25*)
phenyl(3-pyridinyl)methanone	O=C(c1ccccc1)c1cccnc1	RYMBAPVTUHZCNF-UHFFFAOYSA-N	6.4	(*25*)
methyl nicotinate	COC(=O)c1cccnc1	YNBADRVTZLEFNH-UHFFFAOYSA-N	6.4	(*25*)
4-chloropyridine	Clc1ccncc1	PVMNPAUTCMBOMO-UHFFFAOYSA-N	6.5	(*25*)
n,n-dimethyl-2-pyridinamine	CN(C)c1ccccn1	PSHKMPUSSFXUIA-UHFFFAOYSA-N	6.6	(*25*)
2,6-diethylpyridine	CCc1cccc(CC)n1	WHTDCOSHHMXZNE-UHFFFAOYSA-N	6.6	(*21*)
2-vinylpyridine	C=Cc1ccccn1	KGIGUEBEKRSTEW-UHFFFAOYSA-N	6.7	(*25*)
1-(4-pyridinyl)ethanone	CC(=O)c1ccncc1	WMQUKDQWMMOHSA-UHFFFAOYSA-N	6.7,6.4	(*10*)(*25*)
2-ethylpyridine	CCc1ccccn1	NRGGMCIBEHEAIL-UHFFFAOYSA-N	6.8,7.4	(*21*)(*25*)
2-isopropylpyridine	CC(C)c1ccccn1	PFYPDUUXDADWKC-UHFFFAOYSA-N	7.0	(*25*)
1,7-phenanthroline	c1cnc2c(c1)ccc1ncccc12	OZKOMUDCMCEDTM-UHFFFAOYSA-N	7.2	(*25*)
phenanthridine	c1ccc2c(c1)cnc1ccccc12	RDOWQLZANAYVLL-UHFFFAOYSA-N	7.2	(*25*)
2-butylpyridine	CCCCc1ccccn1	ADSOSINJPNKUJK-UHFFFAOYSA-N	7.2	(*25*)
pyridine	c1ccncc1	JUJWROOIHBZHMG-UHFFFAOYSA-N	7.2,7.1	(*23*)(*21*)(*10*)(*25*)(*20*)

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
2,6-dimethylpyridine	Cc1cccc(C)n1	OISVCGZHLKNMSJ-UHFFFAOYSA-N	7.2,7.8	(*21*)(*25*)
quinoline	c1ccc2ncccc2c1	SMWDFEZZVXVKRB-UHFFFAOYSA-N	7.3,7.1	(*23*)(*21*)(*25*)
4-vinylpyridine	C=Cc1ccncc1	KFDVPJUYSDEJTH-UHFFFAOYSA-N	7.4	(*25*)
4-phenylpyridine	c1ccc(-c2ccncc2)cc1	JVZRCNQLWOELDU-UHFFFAOYSA-N	7.4	(*25*)
acridine	c1ccc2nc3ccccc3cc2c1	DZBUGLKDJFMEHC-UHFFFAOYSA-N	7.4	(*25*)
isoquinoline	c1ccc2cnccc2c1	AWJUIBRHMBBTKR-UHFFFAOYSA-N	7.4	(*23*)(*25*)
4-isopropylpyridine	CC(C)c1ccncc1	FRGXNJWEDDQLFH-UHFFFAOYSA-N	7.4	(*21*)(*21*)
4-ethylpyridine	CCc1ccncc1	VJXRKZJMGVSXPX-UHFFFAOYSA-N	7.4,7.7	(*21*)(*25*)
4-(2-methyl-2-propanyl)pyridine	CC(C)(C)c1ccncc1	YSHMQTRICHYLGF-UHFFFAOYSA-N	7.4,7.7	(*21*)(*25*)
3-ethylpyridine	CCc1cccnc1	MFEIKQPHQINPRI-UHFFFAOYSA-N	7.5	(*25*)
3-methylpyridine	Cc1cccnc1	ITQTTZVARXURQS-UHFFFAOYSA-N	7.5,7.0	(*23*)(*21*)(*25*)
1,8-naphthyridine	C1=CC2=C(N=C1)N=CC=C2	FLBAYUMRQUHISI-UHFFFAOYSA-N	7.5	(*26*)
2-methylpyridine	Cc1ccccn1	BSKHPKMHTQYZBB-UHFFFAOYSA-N	7.6,7.1	(*23*)(*21*)(*25*)
n-methyl-2-pyridinamine	CNc1ccccn1	SVEUVITYHIHZQE-UHFFFAOYSA-N	7.7	(*25*)
3-(1-methyl-2-pyrrolidinyl)pyridine	CN1CCC[C@H]1c1cccnc1	SNICXCGAKADSCV-JTQLQIEISA-N	7.7	(*21*)
5,6,7,8-tetrahydroquinolin-8-one	C1CC(C2=C(C1)C=CC=N2)=O	JIAKIQWNYAZUJD-UHFFFAOYSA-N	7.7	(*26*)
4-methylpyridine	Cc1ccncc1	FKNQCJSGGFJEIZ-UHFFFAOYSA-N	7.7,7.4	(*23*)(*21*)(*25*)
2-pyridinamine	Nc1ccccn1	ICSNLGPSRYBMBD-UHFFFAOYSA-N	7.8	(*25*)
4-methoxypyridine	COc1ccncc1	XQABVLBGNWBWIV-UHFFFAOYSA-N	7.8	(*25*)
2,4,6-trimethylpyridine	Cc1cc(C)nc(C)c1	BWZVCCNYKMEVEX-UHFFFAOYSA-N	7.8,8.1	(*21*)(*25*)
3-aminopyridine	Nc1cccnc1	CUYKNJBYIJFRCU-UHFFFAOYSA-N	7.9	(*25*)
1,10-phenanthroline	c1cc2ccc3cccnc3c2nc1	DGEZNRSVGBDHLK-UHFFFAOYSA-N	7.9	(*26*)
2,4-dimethylpyridine	Cc1ccnc(C)c1	JYYNAJVZFGKDEQ-UHFFFAOYSA-N	8.0,7.2	(*23*)(*21*)
3,4-dimethylpyridine	Cc1ccncc1C	NURQLCJSMXZBPC-UHFFFAOYSA-N	8.0	(*10*)(*25*)
3,5-dimethylpyridine	Cc1cncc(C)c1	HWWYDZCSSYKIAD-UHFFFAOYSA-N	8.0	(*23*)(*25*)
n,n-dimethyl-9-acridinamine	CN(C)c1c2ccccc2nc2ccccc12	JIBRFXMUEQDPGO-UHFFFAOYSA-N	8.2	(*25*)
9-(n,n-dimethylamino)acridine	CN(C)c1cccc2cc3ccccc3nc12	XFRSYDKTYAUVAW-UHFFFAOYSA-N	8.2	(*25*)
n,n-dimethyl-4-quinolinamine	CN(C)c1ccnc2ccccc12	SMNMEJQTBGWHLI-UHFFFAOYSA-N	8.5	(*25*)
n,n-dimethyl-3-pyridinamine	CN(C)c1cccnc1	JEDHEXUPBRMUMB-UHFFFAOYSA-N	8.5	(*25*)
4(1h)-pyridinimine	Nc1ccncc1	NUKYPUAOHBNCPY-UHFFFAOYSA-N	8.7	(*23*)
4-(1-methylhydrazino)pyridine	CN(N)c1ccncc1	XWEFKJNJSVXMOD-UHFFFAOYSA-N	8.8	(*25*)
4-(4-methyl-1-piperidinyl)pyridine	CC1CCN(c2ccncc2)CC1	FGWQRDGADJMULT-UHFFFAOYSA-N	9.0	(*25*)
n-methyl-4-pyridinamine	CNc1ccncc1	LSCYTCMNCWMCQE-UHFFFAOYSA-N	9.0	(*23*)
4-(1-piperidinyl)pyridine	c1cc(N2CCCCC2)ccn1	MTPBUCCXRGSDCR-UHFFFAOYSA-N	9.0	(*25*)
n,n-dimethyl-4-pyridinamine	CN(C)c1ccncc1	VHYFNPMBLIVWCW-UHFFFAOYSA-N	9.3,9.5	(*23*)(*21*)(*25*)(*20*)
n,n-diethyl-4-pyridinamine	CCN(CC)c1ccncc1	ODKLEQPZOCJQMT-UHFFFAOYSA-N	9.5	(*25*)
4-(1-pyrrolidinyl)pyridine	c1cc(N2CCCC2)ccn1	RGUKYNXWOWSRET-UHFFFAOYSA-N	9.6	(*23*)(*25*)

3.2.7 SP2-N

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
acetone o-phenyloxime	CC(C)=NOc1ccccc1	QRPMWVNREKTPOV-UHFFFAOYSA-N	4.8	(*10*)
(1e)-cyclohex-3-en-1-one o-decyloxime	CCCCCCCCCCO/N=C1/CC=CCC1	RPYZIZAINHSCRS-MSUUIHNZSA-N	5.5	(*10*)
(1e)-n,n'-diphenylethanimidamide	C/C(=N \c1ccccc1)Nc1ccccc1	CLWIJUQLAFJNOF-UHFFFAOYSA-N	6.7	(*20*)
n,n-dimethyl-n'-phenylimidoformamide	CN(C)/C=N/c1ccccc1	SRPCLECGIYMIMN-CSKARUKUSA-N	7.3	(*21*)
2-dimethylamino-3,3-dimethylazirine	CN(C)C1=NC1(C)C	OQEINIBVOPRVOG-UHFFFAOYSA-N	8.6	(*21*)
5-methyl-3,4-dihydro-2h-pyrrole	CC1=NCCC1	CTSZPNIMMLSKDV-UHFFFAOYSA-N	8.8	(*20*)
n,n-dimethylimidoformamide	CN(C)C=N	DSWNRHCOGVRDOE-ONEGZZNKSA-N	10.0	(*21*)
1,1,3,3-tetramethylguanidine	CN(C)C(=N)N(C)C	KYVBNYUBXIEUFW-UHFFFAOYSA-N	10.0,10.2	(*21*)(*20*)

3.2.8 AZOLE

Common Name	Canonical Smiles	InChIKey	β	References
3,5-diphenyl-1,2,4-oxadiazole	c1ccc(-c2noc(-c3ccccc3)n2)cc1	VIZNDSYPXQJMCM-UHFFFAOYSA-N	3.8	(*10*)
2,1,3-benzothiadiazole	c1ccc2nsnc2c1	PDQRQJVPEFGVRK-UHFFFAOYSA-N	4.2	(*10*)
1,2-oxazole	c1cnoc1	CTAPFRYPJLPFDF-UHFFFAOYSA-N	4.7	(*10*)
1,3-oxazole	c1cocn1	ZCQWOFVYLHDMMC-UHFFFAOYSA-N	5.8	(*10*)
1,3-benzothiazole	c1ccc2scnc2c1	IOJUPLGTWVMSFF-UHFFFAOYSA-N	6.1	(*10*)
10,11-dihydro-5h-tetrazolo[1,5-b][2]benzazepine	c1ccc2c(c1)CCc1nnnn1C2	FUNXVDFRBZQHKX-UHFFFAOYSA-N	6.3	(*10*)
1-methyl-1h-benzotriazole	Cn1nnc2ccccc21	HXQHRUJXQJEGER-UHFFFAOYSA-N	6.6	(*10*)
1-benzyl-1h-1,2,4-triazole	c1ccc(Cn2cncn2)cc1	BNWQEHYYXTVKOF-UHFFFAOYSA-N	7.0	(*10*)(*10*)
1-methyl-1h-pyrazole	Cn1cccn1	UQFQONCQIQEYPJ-UHFFFAOYSA-N	7.1	(*10*)(*10*)
2,5-dimethyl-1,3,4-thiadiazole	Cc1nnc(C)s1	JXQGICFGPUAVLJ-UHFFFAOYSA-N	7.2	(*10*)
thiazole	c1cscn1	FZWLAAWBMGSTSO-UHFFFAOYSA-N	7.3	
1-(2-phenylethyl)-1h-1,2,3-triazole	c1ccc(CCn2ccnn2)cc1	GCDVQIPVANUWJO-UHFFFAOYSA-N	7.3	(*10*)
2,4,5-trimethyl-1,3-oxazole	Cc1nc(C)c(C)o1	ZRLDBDZSLLGDOX-UHFFFAOYSA-N	7.5	(*10*)
2-methyl-5-(methylsulfanyl)-1,3,4-t hiadiazole	CSc1nnc(C)s1	NEKCOKJRDOPRSK-UHFFFAOYSA-N	7.5	
5-bromo-1-methyl-1h-imidazole	Cn1cncc1Br	HATLLUIOEIXWGD-UHFFFAOYSA-N	8.0	(*23*)
imidazole	c1c[nH]cn1	RAXXELZNTBOGNW-UHFFFAOYSA-N	8.5	(*23*)
4-butyl-4h-1,2,4-triazole	CCCCn1cnnc1	ZOMKCDYJHAQMCU-UHFFFAOYSA-N	8.7	(*10*)
4-methylimidazole	Cc1c[nH]cn1	XLSZMDLNRCVEIJ-UHFFFAOYSA-N	8.9	(*23*)
1-methyl-1h-imidazole	Cn1ccnc1	MCTWTZJPVLRJOU-UHFFFAOYSA-N	9.1,8.9	(*23*)(*21*)(*10*)(*20*)

3.2.9 N HETEROCYCLE

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
1,3,5-triazine	c1ncncn1	JIHQDMXYYFUGFV-UHFFFAOYSA-N	3.8,4.8	(*25*)(*20*)
5-bromopyrimidine	Brc1cncnc1	GYCPLYCTMDTEPU-UHFFFAOYSA-N	4.4	(*25*)
pyrazine	c1cnccn1	KYQCOXFCLRTKLS-UHFFFAOYSA-N	5.6,5.1	(*21*)(*10*)(*25*)
2,5-dimethylpyrazine	Cc1cnc(C)cn1	LCZUOKDVTBMCMX-UHFFFAOYSA-N	5.9	(*23*)
phenazine	c1ccc2nc3ccccc3nc2c1	PCNDJXKNXGMECE-UHFFFAOYSA-N	6.0	(*25*)
pyrimidine	c1cncnc1	CZPWVGJYEJSRLH-UHFFFAOYSA-N	6.0,5.4,6.1	(*21*)(*10*)(*25*)(*20*)
n,n-dimethyl-2-pyrimidinamine	CN(C)c1ncccn1	OUMGIYIBWRLOAF-UHFFFAOYSA-N	6.2	(*25*)
4,6-dimethylpyrimidine	Cc1cc(C)ncn1	LSBIUXKNVUBKRI-UHFFFAOYSA-N	6.3	(*23*)
quinazoline	c1ccc2ncncc2c1	JWVCLYRUEFBMGU-UHFFFAOYSA-N	6.5	(*25*)
2(1h)-pyrimidinimine	Nc1ncccn1	LJXQPZWIHJMPQQ-UHFFFAOYSA-N	6.9,7.2	(*21*)(*25*)
n,n-dimethyl-5-pyrimidinamine	CN(C)c1cncnc1	JWVNPUBYKCSIKR-UHFFFAOYSA-N	7.2	(*25*)
pyridazine	c1ccnnc1	PBMFSQRYOILNGV-UHFFFAOYSA-N	7.2,6.7	(*21*)(*10*)(*25*)
n,n-dimethyl-4-pyrimidinamine	CN(C)c1ccncn1	MSXIOWULDXZJLX-UHFFFAOYSA-N	7.7	(*25*)
phtalazine	c1ccc2cnncc2c1	LFSXCDWNBUNEEM-UHFFFAOYSA-N	7.4	(*25*)

3.2.10 NITRILE

Common Name	Canonical Smiles	InChIKey	β	References
trichloroacetonitrile	N#CC(Cl)(Cl)Cl	DRUIESSIVFYOMK-UHFFFAOYSA-N	2.3,2.5	(*21*)(*21*)(*27*)(*28*)
pentafluorobenzonitrile	N#Cc1c(F)c(F)c(F)c(F)c1F	YXWJGZQOGXGSSC-UHFFFAOYSA-N	3.1	(*21*)
dichloroacetonitrile	N#CC(Cl)Cl	STZZWJCGRKXEFF-UHFFFAOYSA-N	3.4	(*21*)
propiolonitrile	C#CC#N	LNDJVIYUJOJFSO-UHFFFAOYSA-N	3.7	(*27*)(*28*)
chloroacetonitrile	N#CCCl	RENMDAKOXSCIGH-UHFFFAOYSA-N	3.9,4.1	(*23*)(*21*)(*27*)(*28*)(*10*)
[(cyanocarbonothioyl)imino]dimethane	CN(C)C(=S)C#N	OLJDIRLJSRSJNR-UHFFFAOYSA-N	4.4	(*21*)
4-chlorobenzonitrile	N#Cc1ccc(Cl)cc1	GJNGXPDXRVXSEH-UHFFFAOYSA-N	4.5,4.6	(*23*)(*27*)(*28*)(*10*)
acrylonitrile	C=CC#N	NLHHRLWOUZZQLW-UHFFFAOYSA-N	4.6	(*23*)(*27*)(*28*)
methoxyacetonitrile	COCC#N	QKPVEISEHYYHRH-UHFFFAOYSA-N	4.7	(*10*)
4-fluorobenzonitrile	N#Cc1ccc(F)cc1	AEKVBBNGWBBYLL-UHFFFAOYSA-N	4.7	(*27*)(*28*)
phenylacetonitrile	N#CCc1ccccc1	SUSQOBVLVYHIEX-UHFFFAOYSA-N	4.8	(*21*)
benzonitrile	N#Cc1ccccc1	JFDZBHWFFUWGJE-UHFFFAOYSA-N	4.8,5.0	(*23*)(*21*)(*27*)(*28*)
2-pyridinecarbonitrile	N#Cc1ccccn1	FFNVQNRYTPFDDP-UHFFFAOYSA-N	5.0	(*25*)
2,6-dimethylbenzonitrile	Cc1cccc(C)c1C#N	QSACPWSIIRFHHR-UHFFFAOYSA-N	5.0	(*23*)
3-methylbenzonitrile	Cc1cccc(C#N)c1	BOHCMQZJWOGWTA-UHFFFAOYSA-N	5.0	(*27*)(*28*)
3-butenenitrile	C=CCC#N	SJNALLRHIVGIBI-UHFFFAOYSA-N	5.0	(*23*)
ethyl 4-cyanobenzoate	CCOC(=O)c1ccc(C#N)cc1	JLSSWDFCYXSLQX-UHFFFAOYSA-N	5.1	(*29*)
3-methoxypropanenitrile	COCCC#N	OOWFYDWAMOKVSF-UHFFFAOYSA-N	5.1	(*10*)
acetonitrile	CC#N	WEVYAHXRMPXWCK-UHFFFAOYSA-N	5.1,5.2	(*23*)(*21*)(*27*)(*28*)(*20*)
valeronitrile	CCCCC#N	RFFFKMOABOFIDF-UHFFFAOYSA-N	5.2	(*21*)
4-acetylbenzonitrile	CC(=O)c1ccc(C#N)cc1	NLPHXWGWBKZSJC-UHFFFAOYSA-N	5.2	(*30*)
1-cyanobutane	CCCC#N	KVNRLNFWIYMESJ-UHFFFAOYSA-N	5.2	(*21*)
4-methoxybenzonitrile	COc1ccc(C#N)cc1	XDJAAZYHCCRJOK-UHFFFAOYSA-N	5.2	(*23*)(*27*)(*28*)
propiononitrile	CCC#N	FVSKHRXBFJPNKK-UHFFFAOYSA-N	5.2	(*23*)(*21*)
2-methylpropanenitrile	CC(C)C#N	LRDFRRGEGBBSRN-UHFFFAOYSA-N	5.3	(*23*)
pivalonitrile	CC(C)(C)C#N	JAMNHZBIQDNHMM-UHFFFAOYSA-N	5.3,5.2	(*23*)(*21*)(*27*)(*28*)
cyclopropanecarbonitrile	N#CC1CC1	AUQDITHEDVOTCU-UHFFFAOYSA-N	5.4	(*27*)(*28*)
4-(dimethylamino)benzonitrile	CN(C)c1ccc(C#N)cc1	JYMNQRQQBJIMCV-UHFFFAOYSA-N	5.8	(*23*)(*27*)(*28*)
(2e)-3-(dimethylamino)acrylonitrile	CN(C)/C=C/C#N	ZKKBIZXAEDFPNL-HWKANZROSA-N	6.8	(*23*)(*27*)(*28*)

3.2.11 OTHER SP-N

Common Name	Canonical Smiles	InChIKey	β	References
cyanic bromide	N#CBr	ATDGTVJJHBUTRL-UHFFFAOYSA-N	3.5	(*27*)(*28*)
ethyl thiocyanate	CCSC#N	WFCLYEAZTHWNEH-UHFFFAOYSA-N	4.4	(*21*)
methyl thiocyanate	CSC#N	VYHVQEYOFIYNJP-UHFFFAOYSA-N	4.7,4.3	(*23*)(*21*)(*27*)(*28*)
phenyl cyanate	N#COc1ccccc1	CWHFDTWZHFRTAB-UHFFFAOYSA-N	4.8	(*27*)(*28*)
diphenylphosphinous cyanide	N#CP(c1ccccc1)c1ccccc1	CSTJIJYJEWKYGH-UHFFFAOYSA-N	4.8	(*21*)(*21*)
trimethylsilanecarbonitrile	C[Si](C)(C)C#N	LEIMLDGFXIOXMT-UHFFFAOYSA-N	5.1	(*27*)(*28*)
cyanamide	N#CN	XZMCDFZZKTWFGF-UHFFFAOYSA-N	5.6	(*23*)
dimethylcyanamide	CN(C)C#N	OAGOUCJGXNLJNL-UHFFFAOYSA-N	6.5,6.4	(*23*)(*21*)(*27*)(*28*)(*10*)
1-piperidinecarbonitrile	N#CN1CCCCC1	NVPICXQHSYQKGM-UHFFFAOYSA-N	6.6	(*23*)
diethylcyanamide	CCN(C#N)CC	ZZTSQZQUWBFTAT-UHFFFAOYSA-N	6.7	(*23*)(*20*)
n'-cyano-n,n-dimethylimidoformamide	CN(C)/C=N/C#N	QFHAGCRNENPASY-GQCTYLIASA-N	7.7	(*23*)(*27*)(*28*)
1-cyano-2-methyl-3-propylguanidine	CCCN/C(=N/C#N)NC	CYFPVACSJLXVCA-UHFFFAOYSA-N	7.9	(*10*)
n'-cyano-n,n-dimethylacetamidine	C/C(=N/C#N)N(C)C	YEEMHJNIVXNCSN-ALCCZGGFSA-N	8.0	(*27*)(*28*)
trimethylammoniocyanamidate	C[N+](C)(C)[N-]C#N	RTJGTTXUCVCPIQ-UHFFFAOYSA-N	10.3	(*27*)(*28*)

3.3 ARSENIC

Common Name	Canonical Smiles	InChIKey	β	References
triphenylarsine	c1ccc([As](c2ccccc2)c2ccccc2)cc1	BPLUKJNHPBNVQL-UHFFFAOYSA-N	3.6	(*21*)

3.4 OXYGEN

3.4.1 WATER

Common Name	Canonical Smiles	InChIKey	β	References
water	O	XLYOFNOQVPJJNP-UHFFFAOYSA-N	4.5	(*21*)(*20*)(*16*)

3.4.2 ALCOHOL

Common Name	Canonical Smiles	InChIKey	β	References
1,1,1,3,3,3-hexafluoro-2-propanol	OC(C(F)(F)F)C(F)(F)F	BYEAHWXPCBROCE-UHFFFAOYSA-N	0.9	(*21*)(*16*)
2,2,2-trifluoroethanol	OCC(F)(F)F	RHQDFWAXVIIEBN-UHFFFAOYSA-N	2.5	(*21*)(*16*)
2,2,2-trichloroethanol	OCC(Cl)(Cl)Cl	KPWDGTGXUYRARH-UHFFFAOYSA-N	2.8	(*21*)(*16*)
prop-2-yn-1-ol	C#CCO	TVDSBUOJIPERQY-UHFFFAOYSA-N	3.7	(*21*)(*16*)
2-chloroethanol	OCCCl	SZIFAVKTNFCBPC-UHFFFAOYSA-N	4.2	(*21*)(*16*)
2-bromoethanol	OCCBr	LDLCZOVUSADOIV-UHFFFAOYSA-N	4.2	(*21*)(*16*)
2-fluoroethanol	OCCF	GGDYAKVUZMZKRV-UHFFFAOYSA-N	4.3	(*21*)(*16*)
2-propen-1-ol	C=CCO	XXROGKLTLUQVRX-UHFFFAOYSA-N	4.8	(*21*)(*16*)
methanol	CO	OKKJLVBELUTLKV-UHFFFAOYSA-N	4.8,4.9	(*21*)(*20*)(*16*)
phenylmethanol	OCc1ccccc1	WVDDGKGOMKODPV-UHFFFAOYSA-N	4.9	(*21*)(*16*)
ethanol	CCO	LFQSCWFLJHTTHZ-UHFFFAOYSA-N	5.2	(*21*)(*16*)
2-phenylethanol	OCCc1ccccc1	WRMNZCZEMHIOCP-UHFFFAOYSA-N	5.3	(*21*)(*16*)
ethylene glycol	OCCO	LYCAIKOWRPUZTN-UHFFFAOYSA-N	5.3	(*21*)(*16*)
1-propanol	CCCO	BDERNNFJNOPAEC-UHFFFAOYSA-N	5.3	(*21*)(*16*)
butan-1-ol	CCCCO	LRHPLDYGYMQRHN-UHFFFAOYSA-N	5.4	(*21*)(*16*)
octan-1-ol	CCCCCCCCO	KBPLFHHGFOOTCA-UHFFFAOYSA-N	5.4	(*21*)(*16*)
2-propanol	CC(C)O	KFZMGEQAYNKOFK-UHFFFAOYSA-N	5.5	(*21*)(*16*)
cyclohexanol	OC1CCCCC1	HPXRVTGHNJAIIH-UHFFFAOYSA-N	5.6	(*21*)(*16*)
2-methyl-2-propanol	CC(C)(C)O	DKGAVHZHDRPRBM-UHFFFAOYSA-N	5.7	(*21*)(*16*)
adamantan-1-ol	O[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2	VLLNJDMHDJRNFK-CHIWXEEVSA-N	5.9	(*21*)(*16*)

3.4.3 PHENOL

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
pentafluorophenol	Oc1c(F)c(F)c(F)c(F)c1F	XBNGYFFABRKICK-UHFFFAOYSA-N	0.8	(*21*)(*16*)
3-(trifluoromethyl)phenol	Oc1cccc(C(F)(F)F)c1	UGEJOEBBMPOJMT-UHFFFAOYSA-N	2.3	(*21*)(*16*)
4-fluorophenol	Oc1ccc(F)cc1	RHMPLDJJXGPMEX-UHFFFAOYSA-N	2.8	(*21*)(*16*)
phenol	Oc1ccccc1	ISWSIDIOOBJBQZ-UHFFFAOYSA-N	2.9	(*21*)(*20*)(*16*)
p-cresol	Cc1ccc(O)cc1	IWDCLRJOBJJRNH-UHFFFAOYSA-N	3.1	(*21*)(*16*)
m-cresol	Cc1cccc(O)c1	RLSSMJSEOOYNOY-UHFFFAOYSA-N	3.1	(*21*)(*16*)

3.4.4 BETAINE

Common Name	Canonical Smiles	InChIKey	β	References
reichardt's dye	[O-]c1c(-c2ccccc2)cc(-[n+]2 c(-c3ccccc3)cc(-c3ccccc3)cc2-c2cccc c2)cc1-c1ccccc1	UWOVWIIOKHRNKU-UHFFFAOYSA-N	14.0	(*5*)

3.4.5 ETHER

Common Name	Canonical Smiles	InChIKey	β	References
1,1,1,3,3,3-hexafluoro-isopropyl me thyl ether	COC(C(F)(F)F)C(F)(F)F	VNXYDFNVQBICRO-UHFFFAOYSA-N	2.2	(*22*)
dichloromethyl methyl ether	COC(Cl)Cl	GRTGGSXWHGKRSB-UHFFFAOYSA-N	2.9	(*22*)
diphenyl ether	c1ccc(Oc2ccccc2)cc1	USIUVYZYUHIAEV-UHFFFAOYSA-N	3.1	(*21*)
1,3,5-trioxane	C1OCOCO1	BGJSXRVXTHVRSN-UHFFFAOYSA-N	3.1	(*22*)
anisole	COc1ccccc1	RDOXTESZEPMUJZ-UHFFFAOYSA-N	3.3	(*20*)
ethyl vinyl ether	C=COCC	FJKIXWOMBXYWOQ-UHFFFAOYSA-N	3.3	(*22*)
tetramethyl orthocarbonate	COC(OC)(OC)OC	AHJWSRRHTXRLAQ-UHFFFAOYSA-N	3.6	(*22*)
bis(2-chloroethyl) ether	ClCCOCCCl	ZNSMNVMLTJELDZ-UHFFFAOYSA-N	3.7	(*22*)
3,4-dihydro-2h-pyran	C1=COCCC1	BUDQDWGNQVEFAC-UHFFFAOYSA-N	4.0	(*22*)
1,3-dioxolane	C1COCO1	WNXJIVFYUVYPPR-UHFFFAOYSA-N	4.1,4.7	(*22*)(*10*)
2,3-dihydrofuran	C1=COCC1	JKTCBAGSMQIFNL-UHFFFAOYSA-N	4.2	(*22*)
2-chloroethyl ethyl ether	CCOCCCl	GPTVQTPMFOLLOA-UHFFFAOYSA-N	4.3	(*22*)
trimethoxy orthoformate	COC(OC)OC	PYOKUURKVVELLB-UHFFFAOYSA-N	4.3	(*22*)
dimethoxymethane	COCOC	NKDDWNXOKDWJAK-UHFFFAOYSA-N	4.4	(*22*)
1,3-dioxane	C1COCOC1	VDFVNEFVBPFDSB-UHFFFAOYSA-N	4.5	(*22*)
diallyl ether	C=CCOCC=C	ATVJXMYDOSMEPO-UHFFFAOYSA-N	4.6	(*22*)
1,4-thioxane	C1CSCCO1	JBYHSSAVUBIJMK-UHFFFAOYSA-N	4.7	(*10*)
di-tert-butyl ether	CC(C)(C)OC(C)(C)C	AQEFLFZSWDEAIP-UHFFFAOYSA-N	4.7,4.5	(*22*)(*21*)
dibenzyl ether	c1ccc(COCc2ccccc2)cc1	MHDVGSVTJDSBDK-UHFFFAOYSA-N	4.7,4.6	(*22*)(*21*)
1,4-dioxane	C1COCCO1	RYHBNJHYFVUHQT-UHFFFAOYSA-N	4.7,4.8,5.4	(*22*)(*21*)(*20*)
dibutyl ether	CCCCOCCCC	DURPTKYDGMDSBL-UHFFFAOYSA-N	5.0,4.9	(*22*)(*21*)
dimethyl ether	COC	LCGLNKUTAGEVQW-UHFFFAOYSA-N	5.1	(*21*)

Common Name	Canonical Smiles	InChIKey	β	References
n-propylethylether	CCCOCC	NVJUHMXYKCUMQA-UHFFFAOYSA-N	5.2	(*21*)
dipropyl ether	CCCOCCC	POLCUAVZOMRGSN-UHFFFAOYSA-N	5.2	(*21*)
diethyl ether	CCOCC	RTZKZFJDLAIYFH-UHFFFAOYSA-N	5.3	(*22*)(*21*)(*20*)
1,2-dimethoxyethane	COCCOC	XTHFKEDIFFGKHM-UHFFFAOYSA-N	5.3,5.8	(*22*)(*10*)
1,3-oxathiane	C1COCSC1	QVFHFKPGBODJJB-UHFFFAOYSA-N	5.4	
dipentyl ether	CCCCCOCCCCC	AOPDRZXCEAKHHW-UHFFFAOYSA-N	5.4	(*21*)
1,2-diethoxyethane	CCOCCOCC	LZDKZFUFMNSQCJ-UHFFFAOYSA-N	5.5	(*22*)
diisopropyl ether	CC(C)OC(C)C	ZAFNJMIOTHYJRJ-UHFFFAOYSA-N	5.5,5.3	(*22*)(*21*)
tert-butyl ethyl ether	CCOC(C)(C)C	NUMQCACRALPSHD-UHFFFAOYSA-N	5.5,5.7	(*22*)(*21*)
15-crown-5	C1COCCOCCOCCOCCO1	VFTFKUDGYRBSAL-UHFFFAOYSA-N	5.6	(*22*)
12-crown-4	C1COCCOCCOCCO1	XQQZRZQVBFHBHL-UHFFFAOYSA-N	5.6	(*22*)
tert-butyl methyl ether	COC(C)(C)C	BZLVMXJERCGZMT-UHFFFAOYSA-N	5.7,5.4	(*22*)(*10*)
18-crown-6	C1COCCOCCOCCOCCOCCO1	XEZNGIUYQVAUSS-UHFFFAOYSA-N	5.7,7.5	(*22*)(*20*)
tetrahydropyran	C1CCOCC1	DHXVGJBLRPWPCS-UHFFFAOYSA-N	5.8,5.5	(*22*)(*21*)
tetrahydrofuran	C1CCOC1	WYURNTSHIVDZCO-UHFFFAOYSA-N	5.9	(*22*)(*21*)(*20*)
2-methyltetrahydrofuran	C[C@@H]1CCCO1	JWUJQDFVADABEY-RXMQYKEDSA-N	6.0	(*22*)
cineole	CC1(C)O[C@]2(C)CC[C@H]1CC2	WEEGYLXZBRQIMU-WAAGHKOSSA-N	6.1,5.9	(*22*)(*21*)
2,2,5,5-tetramethyltetrahyrdofuran	CC1(C)CCC(C)(C)O1	BBLDTXFLAHKYFJ-UHFFFAOYSA-N	6.2	(*22*)

3.4.6 EPOXIDE

Common Name	Canonical Smiles	InChIKey	β	References
epichlorhydrin	ClC[C@H]1CO1	BRLQWZUYTZBJKN-VKHMYHEASA-N	4.0	(*22*)
propylene oxide	C[C@H]1CO1	GOOHAUXETOMSMM-VKHMYHEASA-N	5.2	(*22*)
cyclohexene oxide	C1CC[C@H]2O[C@H]2C1	ZWAJLVLEBYIOTI-OLQVQODUSA-N	5.6	(*22*)
ethylene oxide	C1COC1	AHHWIHXENZJRFG-UHFFFAOYSA-N	6.1,6.2	(*22*)(*21*)
2,3-diadamant-2-yl oxirane	C1[C@H]2C[C@H]3C[C@@H]1 C[C@@H](C2)[C@]31O[C@@] 12[C@@H]1C[C@H]3C[C@@H](C1)C[C@@H]2C3	QDDLRYYYCREGPC-DTJXOCLSSA-N	6.3	(*22*)

3.4.7 PEROXIDE

Common Name	Canonical Smiles	InChIKey	β	References
tert-butyl peroxide	CC(C)(C)OOC(C)(C)C	LSXWFXONGKSEMY-UHFFFAOYSA-N	3.4	(*22*)
ascaridole	CC(C)[C@@]12C=C[C@@](C)(CC1)OO2	MGYMHQJELJYRQS-VHSXEESVSA-N	5.1	(*22*)

3.4.8 PEROXY ACID

Common Name	Canonical Smiles	InChIKey	β	References
3,4-diadamantyl-2-yl-dioxetan	C1[C@H]2C[C@H]3C[C@@H]1 C[C@@H](C2)[C@]31OO[C@@] 12[C@@H]1C[C@H]3C[C@@H](C1)C[C@@H]2C3	OLJVAWRLTPGYQL-DTJXOCLSSA-N	4.5	(*22*)

3.4.9 SILOXANE

Common Name	Canonical Smiles	InChIKey	β	References
hexamethyldisiloxane	C[Si](C)(C)O[Si](C)(C)C	UQEAIHBTYFGYIE-UHFFFAOYSA-N	1.9	(*22*)

3.4.10 ALDEHYDE

Common Name	Canonical Smiles	InChIKey	β	References
4-chlorobenzaldehyde	O=Cc1ccc(Cl)cc1	AVPYQKSLYISFPO-UHFFFAOYSA-N	4.5	(*30*)
acetaldehyde	CC=O	IKHGUXGNUITLKF-UHFFFAOYSA-N	4.5	(*30*)
propanaldehyde	CCC=O	NBBJYMSMWIIQGU-UHFFFAOYSA-N	4.6	(*21*)
octanaldehyde	CCCCCCCC=O	NUJGJRNETVAIRJ-UHFFFAOYSA-N	4.6	(*21*)
decanaldehyde	CCCCCCCCCC=O	KSMVZQYAVGTKIV-UHFFFAOYSA-N	4.7	(*21*)
butanaldehyde	CCCC=O	ZTQSAGDEMFDKMZ-UHFFFAOYSA-N	4.7	(*21*)
benzaldehyde	O=Cc1ccccc1	HUMNYLRZRPPJDN-UHFFFAOYSA-N	4.9,4.8	(*21*)(*30*)(*20*)
2-methoxybenzaldehyde	COc1ccccc1C=O	PKZJLOCLABXVMC-UHFFFAOYSA-N	5.5	(*30*)
4-methoxybenzaldehyde	COc1ccc(C=O)cc1	ZRSNZINYAWTAHE-UHFFFAOYSA-N	5.5	(*30*)
(2e)-3-phenylacrylaldehyde	O=C/C=C/c1ccccc1	KJPRLNWUNMBNBZ-QPJJXVBHSA-N	5.6	(*30*)
4-(dimethylamino)benzaldehyde	CN(C)c1ccc(C=O)cc1	BGNGWHSBYQYVRX-UHFFFAOYSA-N	6.5	(*30*)

3.4.11 KETONE

Common Name	Canonical Smiles	InChIKey	β	References
hexafluoropropanone	O=C(C(F)(F)F)C(F)(F)F	VBZWSGALLODQNC-UHFFFAOYSA-N	2.6	(*21*)
1,1,1-trifluoropropan-2-one	CC(=O)C(F)(F)F	FHUDAMLDXFJHJE-UHFFFAOYSA-N	2.9	(*30*)
1,1,1-trichloropropan-2-one	CC(=O)C(Cl)(Cl)Cl	SMZHKGXSEAGRTI-UHFFFAOYSA-N	3.1	(*30*)
1,1-dichloropropan-2-one	CC(=O)C(Cl)Cl	CSVFWMMPUJDVKH-UHFFFAOYSA-N	3.6	(*30*)
biacetyl	CC(=O)C(C)=O	QSJXEFYPDANLFS-UHFFFAOYSA-N	4.2	(*30*)
1,3-dichloroacetone	O=C(CCl)CCl	SUNMBRGCANLOEG-UHFFFAOYSA-N	4.2,3.8	(*21*)(*30*)
1,4-benzoquinone	O=C1C=CC(=O)C=C1	AZQWKYJCGOJGHM-UHFFFAOYSA-N	4.2,4.9	(*21*)(*30*)
chloropropan-2-one	CC(=O)CCl	BULLHNJGPPOUOX-UHFFFAOYSA-N	4.5	(*30*)
1-(3-nitrophenyl)ethanone	CC(=O)c1cccc([N+](=O)[O-])c1	ARKIFHPFTHVKDT-UHFFFAOYSA-N	4.6	(*30*)
3-butyn-2-one	C#CC(C)=O	XRGPFNGLRSIPSA-UHFFFAOYSA-N	4.6	(*30*)
1-[3-(trifluoromethyl)phenyl]ethanone	CC(=O)c1cccc(C(F)(F)F)c1	ABXGMGUHGLQMAW-UHFFFAOYSA-N	4.7	(*30*)
benzil	O=C(C(=O)c1ccccc1)c1ccccc1	WURBFLDFSFBTLW-UHFFFAOYSA-N	4.7	(*30*)
1-[4-(trifluoromethyl)phenyl]ethanone	CC(=O)c1ccc(C(F)(F)F)cc1	HHAISVSEJFEWBZ-UHFFFAOYSA-N	4.8	(*30*)
1-(3-chlorophenyl)ethanone	CC(=O)c1cccc(Cl)c1	UUWJBXKHMMQDED-UHFFFAOYSA-N	4.9	(*30*)
1-(3-fluorophenyl)ethanone	CC(=O)c1cccc(F)c1	HCEKGPAHZCYRBZ-UHFFFAOYSA-N	4.9	(*30*)
1-(4-chlorophenyl)ethanone	CC(=O)c1ccc(Cl)cc1	BUZYGTVTZYSBCU-UHFFFAOYSA-N	5.1	(*30*)
acetyl acetone	CC(=O)CC(C)=O	YRKCREAYFQTBPV-UHFFFAOYSA-N	5.1	(*30*)
1-(2-chlorophenyl)ethanone	CC(=O)c1ccccc1Cl	ZDOYHCIRUPHUHN-UHFFFAOYSA-N	5.1	(*30*)
3-pentanone	CCC(=O)CC	FDPIMTJIUBPUKL-UHFFFAOYSA-N	5.2,5.6,5.4	(*21*)(*30*)(*10*)
1,3-diphenylacetone	O=C(Cc1ccccc1)Cc1ccccc1	YFKBXYGUSOXJGS-UHFFFAOYSA-N	5.3	(*30*)
9,10-phenanthrequinone	O=C1C(=O)c2ccccc2-c2ccccc21	YYVYAPXYZVYDHN-UHFFFAOYSA-N	5.3	(*30*)
dimesitylmethanone	Cc1cc(C)c(C(=O)c2c(C)cc(C)cc2C)c(C)c1	SKMUIZHHMAPKIV-UHFFFAOYSA-N	5.3	(*30*)
cyclobutanone	O=C1CCC1	SHQSVMDWKBRBGB-UHFFFAOYSA-N	5.3	(*30*)
1-(4-fluoro-3-methoxyphenyl)ethanone	COc1cc(C(C)=O)ccc1F	PFEGFUCYOHBDJF-UHFFFAOYSA-N	5.3	(*30*)
4-fluoroacetophenone	CC(=O)c1ccc(F)cc1	ZDPAWHACYDRYIW-UHFFFAOYSA-N	5.3	(*30*)
benzophenone	O=C(c1ccccc1)c1ccccc1	RWCCWEUUXYIKHB-UHFFFAOYSA-N	5.3,5.4	(*21*)(*30*)
4-methyl-2-pentanone	CC(=O)CC(C)C	NTIZESTWPVYFNL-UHFFFAOYSA-N	5.3,5.7	(*21*)(*30*)
3,5-dimethylheptan-4-one	CC[C@H](C)C(=O)[C@H](C)CC	VZXXYILNWWRSGE-OCAPTIKFSA-N	5.4	(*30*)
2,6-dimethylheptan-4-one	CC(C)CC(=O)CC(C)C	PTTPXKJBFFKCEK-UHFFFAOYSA-N	5.4	(*30*)
2,2,4,4-tetramethyl-3-pentanone	CC(C)(C)C(=O)C(C)(C)C	UIQGEWJEWJMQSL-UHFFFAOYSA-N	5.4,5.2	(*21*)(*30*)
3-methyl-2-butanone	CC(=O)C(C)C	SYBYTAAJFKOIEJ-UHFFFAOYSA-N	5.4,5.6	(*21*)(*10*)

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
3,3-dimethyl-2-butanone	CC(=O)C(C)(C)C	PJGSXYOJTGTZAV-UHFFFAOYSA-N	5.4,5.7	(*21*)(*30*)(*30*)
1-(3-methylphenyl)ethanone	CC(=O)c1cccc(C)c1	FSPSELPMWGWDRY-UHFFFAOYSA-N	5.5	(*30*)
2,4-dimethyl-3-pentanone	CC(C)C(=O)C(C)C	HXVNBWAKAOHACI-UHFFFAOYSA-N	5.5	(*30*)
1-(adamantan-1-yl)-2,2-dimethyl-1-p ropanone	CC(C)(C)C(=O)[C@]12C[C@H]3C [C@H](C[C@H](C3)C1)C2	BHTSNYQWLQLLOD-WUQLGEGHSA-N	5.5	(*30*)
9h-fluoren-9-one	O=C1c2ccccc2-c2ccccc21	YLQWCDOCJODRMT-UHFFFAOYSA-N	5.5	(*30*)
1,3-diacetylbenzene	CC(=O)c1cccc(C(C)=O)c1	VCHOFVSNWYPAEF-UHFFFAOYSA-N	5.6	(*30*)
1-(3-methoxyphenyl)ethanone	COc1cccc(C(C)=O)c1	BAYUSCHCCGXLAY-UHFFFAOYSA-N	5.6	(*30*)
heptan-4-one	CCCC(=O)CCC	HCFAJYNVAYBARA-UHFFFAOYSA-N	5.6	(*30*)
9(10h)-anthracenone	O=C1c2ccccc2Cc2ccccc21	RJGDLRCDCYRQOQ-UHFFFAOYSA-N	5.6	(*30*)
1-(2-naphthyl)ethanone	CC(=O)c1ccc2ccccc2c1	XSAYZAUNJMRRIR-UHFFFAOYSA-N	5.6	(*30*)
hexan-3-one	CCCC(=O)CC	PFCHFHIRKBAQGU-UHFFFAOYSA-N	5.6	(*30*)
2-pentanone	CCCC(C)=O	XNLICIUVMPYHGG-UHFFFAOYSA-N	5.6,5.7	(*21*)(*30*)
2-butanone	CCC(C)=O	ZWEHNKRNPOVVGH-UHFFFAOYSA-N	5.6,5.8	(*21*)(*30*)
9h-thioxanthen-9-one	O=c1c2ccccc2sc2ccccc12	YRHRIQCWCFGUEQ-UHFFFAOYSA-N	5.7	(*30*)
cycloundecanone	O=C1CCCCCCCCCC1	UPOSSYJVWXLPTA-UHFFFAOYSA-N	5.7	(*30*)
hexan-2-one	CCCCC(C)=O	QQZOPKMRPOGIEB-UHFFFAOYSA-N	5.7	(*30*)
di(adamantan-1-yl)methanone	O=C([C@]12C[C@H]3C[C@H] (C[C@H](C3)C1)C2)[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2	RGWHHWWMFUXNAX-ICWSVDNISA-N	5.7	(*30*)
acetone	CC(C)=O	CSCPPACGZOOCGX-UHFFFAOYSA-N	5.7	(*21*)(*30*)(*20*)
1-(4-methylphenyl)ethanone	CC(=O)c1ccc(C)cc1	GNKZMNRKLCTJAY-UHFFFAOYSA-N	5.8	(*30*)
3-methylpentan-2-one	CC[C@H](C)C(C)=O	UIHCLUNTQKBZGK-YFKPBYRVSA-N	5.8	(*30*)
cyclododecanone	O=C1CCCCCCCCCCC1	SXVPOSFURRDKBO-UHFFFAOYSA-N	5.8	(*30*)
mesityl oxide	CC(=O)C=C(C)C	SHOJXDKTYKFBRD-UHFFFAOYSA-N	5.8	(*21*)
1-(4-ethylphenyl)ethanone	CCc1ccc(C(C)=O)cc1	NODGRWCMFMEGJH-UHFFFAOYSA-N	5.8	(*30*)
1-[4-(methylsulfanyl)phenyl]ethanone	CSc1ccc(C(C)=O)cc1	JECUZQLBQKNEMW-UHFFFAOYSA-N	5.8	(*30*)
1,1'-(1,4-phenylene)diethanone	CC(=O)c1ccc(C(C)=O)cc1	SKBBQSLSGRSQAJ-UHFFFAOYSA-N	5.8	(*30*)
cyclopentadecanone	O=C1CCCCCCCCCCCCCC1	OSOIQJGOYGSIMF-UHFFFAOYSA-N	5.8	(*30*)
1-(4-isopropylphenyl)ethanone	CC(=O)c1ccc(C(C)C)cc1	PDLCCNYKIIUWHA-UHFFFAOYSA-N	5.8	(*30*)
3-chloro-5,5-dimethyl-2-cyclohexen-1-one	CC1(C)CC(=O)C=C(Cl)C1	PJYTYJGMJDIKEJ-UHFFFAOYSA-N	5.8	(*30*)
cyclohexyl methyl ketone	CC(=O)C1CCCCC1	RIFKADJTWUGDOV-UHFFFAOYSA-N	5.8	(*30*)
1-[4-(2-methyl-2-propanyl)phenyl]et hanone	CC(=O)c1ccc(C(C)(C)C)cc1	UYFJYGWNYQCHOB-UHFFFAOYSA-N	5.8	(*30*)
(4-methoxyphenyl)(phenyl)methanone	COc1ccc(C(=O)c2ccccc2)cc1	SWFHGTMLYIBPPA-UHFFFAOYSA-N	5.9	(*30*)

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
2-methylcyclohexanone	C[C@H]1CCCCC1=O	LFSAPCRASZRSKS-LURJTMIESA-N	5.9	(*30*)
1-phenylethanone	CC(=O)c1ccccc1	KWOLFJPFCHCOCG-UHFFFAOYSA-N	5.9,5.5	(*21*)(*30*)
1-cyclopropylethanone	CC(=O)C1CC1	HVCFCNAITDHQFX-UHFFFAOYSA-N	6.0	(*30*)
1-(adamantan-1-yl)ethanone	CC(=O)[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2	DACIGVIOAFXPHW-CDECOKDKSA-N	6.0	(*30*)
î±,î±'-diphenylbenzotropone	O=c1c(-c2ccccc2)cc2ccccc2cc1-c1ccccc1	GCUVJAHASMTIRG-UHFFFAOYSA-N	6.0	(*30*)
1-(2-methoxyphenyl)ethanone	CC(=[O])c1ccccc1O	DWPLEOPKBWNPQV-UHFFFAOYSA-N	6.0	(*30*)
1-[4-(adamantan-1-yl)phenyl]ethanone	CC(=O)c1ccc([C@]23C[C@H]4C[C@H](C[C@H](C4)C2)C3)cc1	MSPDNPMYZVJMAM-OVMOHIIOSA-N	6.0	(*30*)
1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	CC1(C)[C@@H]2CC[C@@]1(C)C(=O)C2	DSSYKIVIOFKYAU-XCBNKYQSSA-N	6.0	(*30*)
cyclopentanone	O=C1CCCC1	BGTOWKSIORTVQH-UHFFFAOYSA-N	6.0,5.9	(*21*)(*30*)
1-(4-methoxyphenyl)ethanone	COc1ccc(C(C)=O)cc1	NTPLXRHDUXRPNE-UHFFFAOYSA-N	6.0	(*21*)(*30*)
cyclohexanone	O=C1CCCCC1	JHIVVAPYMSGYDF-UHFFFAOYSA-N	6.0,6.2	(*21*)(*30*)(*20*)
(3e)-4-phenyl-3-buten-2-one	CC(=O)/C=C/c1ccccc1	BWHOZHOGCMHOBV-BQYQJAHWSA-N	6.1	(*30*)
9h-xanthen-9-one	O=c1c2ccccc2oc2ccccc12	JNELGWHKGNBSMD-UHFFFAOYSA-N	6.1	(*30*)
piperitone	CC1=CC(=O)[C@H](C(C)C)CC1	YSTPAHQEHQSRJD-VIFPVBQESA-N	6.1	(*21*)
dicyclopropylmethanone	O=C(C1CC1)C1CC1	BIPUHAHGLJKIPK-UHFFFAOYSA-N	6.1	(*30*)
cycloheptanone	O=C1CCCCCC1	CGZZMOTZOONQIA-UHFFFAOYSA-N	6.2	(*30*)
cyclooctanone	O=C1CCCCCCC1	IIRFCWANHMSDCG-UHFFFAOYSA-N	6.3	(*30*)
1-(4-aminophenyl)ethanone	CC(=O)c1ccc(N)cc1	GPRYKVSEZCQIHD-UHFFFAOYSA-N	6.4	(*30*)
bis(4-methoxyphenyl)methanone	COc1ccc(C(=O)c2ccc(OC)cc2)cc1	RFVHVYKVRGKLNK-UHFFFAOYSA-N	6.4	(*30*)
6,8-dimethyl-7h-benzo[7]annulen-7-one	Cc1cc2ccccc2cc(C)c1=O	YVBMXGVGOLXFFS-UHFFFAOYSA-N	6.4	(*30*)
1-[4-(4-morpholinyl)phenyl]ethanone	CC(=O)c1ccc(N2CCOCC2)cc1	AKQWEDMTPCAESO-UHFFFAOYSA-N	6.6	(*30*)
4-(dimethylamino)benzophenone	CN(C)c1ccc(C(=O)c2ccccc2)cc1	BEUGBYXJXMVRFO-UHFFFAOYSA-N	6.8	(*30*)
1-[4-(1-piperidinyl)phenyl]ethanone	CC(=O)c1ccc(N2CCCCC2)cc1	JCMZZYSPSGHBNM-UHFFFAOYSA-N	6.9	(*30*)
3,5,5-trimethyl-2-cyclohexen-1-one	CC1=CC(=O)CC(C)(C)C1	HJOVHMDZYOCNQW-UHFFFAOYSA-N	6.9	(*30*)
4-(dimethylamino)acetophenone	CC(=O)c1ccc(N(C)C)cc1	HUDYANRNMZDQGA-UHFFFAOYSA-N	7.0	(*30*)
4-(diethylamino)acetophenone	CCN(CC)c1ccc(C(C)=O)cc1	HMIBQFXWSUBFTG-UHFFFAOYSA-N	7.1	(*30*)
7h-benzo[7]annulen-7-one	O=c1ccc2ccccc2cc1	VJPAMLCBTIWAHI-UHFFFAOYSA-N	7.2	(*30*)
10-methyl-9(10h)-acridone	Cn1c2ccccc2c(=O)c2ccccc21	XUVKSPPGPPFPQN-UHFFFAOYSA-N	7.3	(*30*)
bis[4-(dimethylamino)phenyl]methanone	CN(C)c1ccc(C(=O)c2ccc(N(C)C)cc2)cc1	VVBLNCFGVYUYGU-UHFFFAOYSA-N	7.3	(*30*)
2-phenyl-4h-chromen-4-one	O=c1cc(-c2ccccc2)oc2ccccc12	VHBFFQKBGNRLFZ-UHFFFAOYSA-N	7.3,7.5	(*21*)(*30*)(*20*)
2,4,6-cycloheptatrien-1-one	O=c1cccccc1	QVWDCTQRORVHHT-UHFFFAOYSA-N	7.4	(*30*)

Common Name	Canonical Smiles	InChIKey	β	References
4h-pyran-4-one	O=c1ccocc1	CVQUWLDCFXOXEN-UHFFFAOYSA-N	7.6	(*30*)
2,3-diphenyl-2-cyclopropen-1-one	O=c1c(-c2ccccc2)c1-c1ccccc1	HCIBTBXNLVOFER-UHFFFAOYSA-N	8.2	(*30*)
bis[4-(diethylamino)phenyl]methanone	CCN(CC)c1ccc(C(=O)c2ccc(N(CC)CC)cc2)cc1	VYHBFRJRBHMIQZ-UHFFFAOYSA-N	8.2	(*30*)
2,6-dimethyl-4h-pyran-4-one	Cc1cc(=O)cc(C)o1	VSYFZULSKMFUJJ-UHFFFAOYSA-N	8.6	(*21*)(*30*)(*20*)
3-(dimethylamino)-5,5-dimethyl-2-cy clohexen-1-one	CN(C)C1=CC(=O)CC(C)(C)C1	XHNTVKASLQLNFM-UHFFFAOYSA-N	9.5	(*30*)
1-methyl-4(1h)-quinolinone	Cn1ccc(=O)c2ccccc21	CSJAXRKDCCWCSJ-UHFFFAOYSA-N	9.8	(*10*)

3.4.12 CARBOXYLIC ACID

Common Name	Canonical Smiles	InChIKey	β	References
butanoic acid	CCCC(=O)O	FERIUCNNQQJTOY-UHFFFAOYSA-N	4.9	(*21*)
benzoic acid	O=C(O)c1ccccc1	WPYMKLBDIGXBTP-UHFFFAOYSA-N	4.9	(*21*)

3.4.13 ESTER

Common Name	Canonical Smiles	InChIKey	β	References
ethyl triflouroacetate	CCOC(=O)C(F)(F)F	STSCVKRWJPWALQ-UHFFFAOYSA-N	3.2	(*29*)
methyl trichloroacetate	COC(=O)C(Cl)(Cl)Cl	VHFUHRXYRYWELT-UHFFFAOYSA-N	3.3	(*29*)
ethyl trichloroacetate	CCOC(=O)C(Cl)(Cl)Cl	SJMLNDPIJZBEKY-UHFFFAOYSA-N	3.4	(*29*)
methyl salicylate	COC(=O)c1ccccc1O	OSWPMRLSEDHDFF-UHFFFAOYSA-N	3.8	(*20*)(*20*)
diethyl oxalate	CCOC(=O)C(=O)OCC	WYACBZDAHNBPPB-UHFFFAOYSA-N	4.5	(*29*)
methyl formate	COC=O	TZIHFWKZFHZASV-UHFFFAOYSA-N	4.5	(*21*)
ethyl propiolate	C#CC(=O)OCC	FMVJYQGSRWVMQV-UHFFFAOYSA-N	4.5	(*29*)
phenylformate	O=COc1ccccc1	GEOWCLRLLWTHDN-UHFFFAOYSA-N	4.5	(*29*)
ethyl formate	CCOC=O	WBJINCZRORDGAQ-UHFFFAOYSA-N	4.5	(*29*)(*20*)
ethyl chloroacetate	CCOC(=O)CCl	VEUUMBGHMNQHGO-UHFFFAOYSA-N	4.6	(*29*)
ethyl flouroacetate	CCOC(=O)CF	VCYZVXRKYPKDQB-UHFFFAOYSA-N	4.7	(*29*)
vinyl acetate	C=CC(=O)OC	BAPJBEWLBFYGME-UHFFFAOYSA-N	4.7	(*21*)
methyl benzoate	COC(=O)c1ccccc1	QPJVMBTYPHYUOC-UHFFFAOYSA-N	4.7,5.0	(*31*)(*29*)
methyl acetate	COC(C)=O	KXKVLQRXCPHEJC-UHFFFAOYSA-N	4.7,5.3	(*21*)(*29*)(*20*)
ethyl 4-bromobenzoate	CCOC(=O)c1ccc(Br)cc1	XZIAFENWXIQIKR-UHFFFAOYSA-N	4.8	(*29*)
diethyl terephthalate	CCOC(=O)c1ccc(C(=O)OCC)cc1	ONIHPYYWNBVMID-UHFFFAOYSA-N	4.8	(*29*)
triacetin	CC(=O)OCC(COC(C)=O)OC(C)=O	URAYPUMNDPQOKB-UHFFFAOYSA-N	4.9	(*29*)
2-oxetanone	O=C1CCO1	VEZXCJBBBCKRPI-UHFFFAOYSA-N	5.0	(*29*)
ethyl 4-fluorobenzoate	CCOC(=O)c1ccc(F)cc1	UMPRJGKLMUDRHL-UHFFFAOYSA-N	5.0	(*29*)
ethyl benzoate	CCOC(=O)c1ccccc1	MTZQAGJQAFMTAQ-UHFFFAOYSA-N	5.0,5.2	(*21*)(*29*)(*20*)
tert-butyl benzoate	CC(C)(C)OC(=O)c1ccccc1	LYDRKKWPKKEMNZ-UHFFFAOYSA-N	5.2	(*29*)
4-methyl-2-oxetanone	C[C@H]1CC(=O)O1	GSCLMSFRWBPUSK-VKHMYHEASA-N	5.2	(*29*)
ethyl acetate	CCOC(C)=O	XEKOWRVHYACXOJ-UHFFFAOYSA-N	5.2,5.4	(*21*)(*29*)
ethyl 3-methylbenzoate	CCOC(=O)c1cccc(C)c1	WSJNYOVBJSOQST-UHFFFAOYSA-N	5.3	(*29*)
ethyl 1-adamantanecarboxylate	CCOC(=O)[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2	SYEXGNJRYPOUSI-DNSLJTBWSA-N	5.4	(*29*)
methyl cyclohexanecarboxylate	COC(=O)C1CCCCC1	ZQWPRMPSCMSAJU-UHFFFAOYSA-N	5.4	(*29*)
methyl cyclohexanecarboxylate	O=C(O)C1CCCCC1	NZNMSOFKMUBTKW-UHFFFAOYSA-N	5.4	(*29*)
ethyl 4-methylbenzoate	CCOC(=O)c1ccc(C)cc1	NWPWRAWAUYIELB-UHFFFAOYSA-N	5.4	(*29*)
ethyl phenylacetate	CCOC(=O)Cc1ccccc1	DULCUDSUACXJJC-UHFFFAOYSA-N	5.4	(*29*)
ethyl 2,2-dimethylpropanoate	CCOC(=O)C(C)(C)C	HHEIMYAXCOIQCJ-UHFFFAOYSA-N	5.4	(*29*)
ethyl isobutyrate	CCOC(=O)C(C)C	WDAXFOBOLVPGLV-UHFFFAOYSA-N	5.5	(*29*)
ethyl propionate	CCOC(=O)CC	FKRCODPIKNYEAC-UHFFFAOYSA-N	5.5	(*29*)

Common Name	Canonical Smiles	InChIKey	β	References
tert-butyl ethanoate	CC(=O)OC(C)(C)C	WMOVHXAZOJBABW-UHFFFAOYSA-N	5.5	(*29*)
ethyl butyrate	CCCC(=O)OCC	OBNCKNCVKJNDBV-UHFFFAOYSA-N	5.5	(*29*)
ethyl 3-methylbutanoate	CCOC(=O)CC(C)C	PPXUHEORWJQRHJ-UHFFFAOYSA-N	5.5	(*29*)
isobutyl acetate	CC(=O)OCC(C)C	GJRQTCIYDGXPES-UHFFFAOYSA-N	5.6	(*29*)
methyl-cyclopropanecarboxylate	COC(=O)C1CC1	PKAHQJNJPDVTDP-UHFFFAOYSA-N	5.6	(*29*)
isopropyl ethanoate	CC(=O)OC(C)C	JMMWKPVZQRWMSS-UHFFFAOYSA-N	5.6	(*29*)
(e)-ethyl cinnamate	CCOC(=O)/C=C/c1ccccc1	KBEBGUQPQBELIU-CMDGGOBGSA-N	5.6	(*29*)
ethyl cyclopropanecarboxylate	CCOC(=O)C1CC1	LDDOSDVZPSGLFZ-UHFFFAOYSA-N	5.6	(*29*)
ethyl 4-methoxybenzoate	CCOC(=O)c1ccc(OC)cc1	FHUODBDRWMIBQP-UHFFFAOYSA-N	5.6	(*29*)
propyl ethanoate	CCCOC(C)=O	YKYONYBAUNKHLG-UHFFFAOYSA-N	5.6	(*29*)
sec-butyl acetate	CC[C@H](C)OC(C)=O	DCKVNWZUADLDEH-YFKPBYRVSA-N	5.6	(*29*)
butyl acetate	CCCCOC(C)=O	DKPFZGUDAPQIHT-UHFFFAOYSA-N	5.6	(*29*)
2h-chromen-2-one	O=c1occc2ccccc12	IQZZFVDIZRWADY-UHFFFAOYSA-N	6.0	(*29*)
dihydro-2(3h)-furanone	O=C1CCCO1	YEJRWHAVMIAJKC-UHFFFAOYSA-N	6.0	(*29*)(*20*)
5-methyldihydro-2(3h)-furanone	C[C@H]1CCC(=O)O1	GAEKPEKOJKCEMS-BYPYZUCNSA-N	6.2	(*29*)
ethyl 4-dimethylaminobenzoate	CCOC(=O)c1ccc(N(C)C)cc1	FZUGPQWGEGAKET-UHFFFAOYSA-N	6.3	(*29*)
tetrahydro-2h-pyran-2-one	O=C1CCCCO1	OZJPLYNZGCXSJM-UHFFFAOYSA-N	6.6	(*29*)
2-oxepanone	O=C1CCCCCO1	PAPBSGBWRJIAAV-UHFFFAOYSA-N	6.7	(*29*)
ethyl 3-(dimethylamino)acrylate	CCOC(=O)/C=C/N(C)C	MVUMJYQUKKUOHO-AATRIKPKSA-N	7.7	(*29*)

3.4.14 ANHYDRIDE

Common Name	Canonical Smiles	InChIKey	β	References
acetic anhydride	CC(=O)OC(C)=O	WFDIJRYMOXRFFG-UHFFFAOYSA-N	6.4	(*21*)

3.4.15 AMIDE

Common Name	Canonical Smiles	InChIKey	β	References
n,n-dimethyl-2,2,2-trifluoroacetamide	CN(C)C(=O)C(F)(F)F	WXBWKMLIVXELSF-UHFFFAOYSA-N	5.4	(*31*)(*20*)
1,1,1-trifluoro-n,n-diethylacetamide	CCN(CC)C(=O)C(F)(F)F	CODXZFSZJFCVBE-UHFFFAOYSA-N	5.5	(*21*)
n,n-dimethyl-2,2,2-trichloroacetamide	CN(C)C(=O)C(Cl)(Cl)Cl	WGBMKQSRUSKSOM-UHFFFAOYSA-N	5.7	(*31*)
1,1,1-trichloro-n,n-diethylacetamide	CCN(CC)C(=O)C(Cl)(Cl)Cl	OIWFZENWZGPLQZ-UHFFFAOYSA-N	5.7	(*21*)
1-methyl-1h-pyrrole-2,5-dione	CN1C(=O)C=CC1=O	SEEYREPSKCQBBF-UHFFFAOYSA-N	5.8	(*10*)
4-nitro-n,n-diphenylbenzamide	O=C(c1ccc([N+](=O)[O-])cc1)N(c1ccccc1)c1ccccc1	HZXRDAIBHPCJLE-UHFFFAOYSA-N	5.9	(*21*)
1-methyl-2,5-pyrrolidinedione	CN1C(=O)CCC1=O	KYEACNNYFNZCST-UHFFFAOYSA-N	6.1	(*20*)
2,2-dichloro-n,n-diethylacetamide	CCN(CC)C(=O)C(Cl)Cl	ZZWJQCJQAXZVOM-UHFFFAOYSA-N	6.2	(*21*)
n,n-diphenylformamide	O=CN(c1ccccc1)c1ccccc1	DCNUQRBLZWSGAV-UHFFFAOYSA-N	6.2	(*31*)
2-chloro-n,n-diphenylacetamide	O=C(CCl)N(c1ccccc1)c1ccccc1	GRIXINIGTYIHSN-UHFFFAOYSA-N	6.2	(*21*)
n-(3-chlorophenyl)pyrrolidin-2-one	O=C1CCCN1c1cccc(Cl)c1	AFHUWZFARIICFX-UHFFFAOYSA-N	6.4	(*21*)
n-(4-chlorophenyl)pyrrolidin-2-one	O=C1CCCN1c1ccc(Cl)cc1	NAIVIVMHCDWBEF-UHFFFAOYSA-N	6.5	(*21*)
n,n-diphenyl-2,2-dimethylpropionamide	CC(C)(C)C(=O)N(c1ccccc1)c1ccccc1	QKZRSIWEFMDUIL-UHFFFAOYSA-N	6.7	(*31*)
n,n-diphenyl-4-methoxybenzamide	COc1ccc(C(=O)N(c2ccccc2)c2ccccc2)cc1	GVALSXYCLDABKT-UHFFFAOYSA-N	6.8	(*31*)
n,n-diphenylbenzamide	O=C(c1ccccc1)N(c1ccccc1)c1ccccc1	RHLIPLVNXYUJQV-UHFFFAOYSA-N	6.8,6.6	(*21*)(*31*)
n,n-diethyl-4-nitrobenzamide	CCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1	JLZWKZDHHREXTA-UHFFFAOYSA-N	6.9	(*21*)
n,n-diphenylpropanamide	CCC(=O)N(c1ccccc1)c1ccccc1	JIRGTCBOQAJBHY-UHFFFAOYSA-N	6.9	(*21*)
n-methylformanilide	CN(C=O)c1ccccc1	JIKUXBYRTXDNIY-UHFFFAOYSA-N	6.9	(*31*)
2-chloro-n,n-dicyclohexylacetamide	O=C(CCl)N(C1CCCCC1)C1CCCCC1	YMBSJQHEFLROIX-UHFFFAOYSA-N	6.9	(*21*)
2-chloro-n,n-dimethylacetamide	CN(C)C(=O)CCl	XBPPLECAZBTMMK-UHFFFAOYSA-N	6.9	(*21*)(*31*)
2-chloro-1-(1-piperidinyl)ethanone	O=C(CCl)N1CCCCC1	NSWLMOHUXYULKL-UHFFFAOYSA-N	7.0	(*21*)
n-(3-methoxyphenyl)pyrrolidin-2-one	COc1cccc(N2CCCC2=O)c1	AKODNVGCZKBUNT-UHFFFAOYSA-N	7.0	(*21*)
n,n-dicyclohexyl-4-nitrobenzamide	O=C(c1ccc([N+](=O)[O-])cc1)N(C1CCCCC1)C1CCCCC1	GXHHFMZALQKUFL-UHFFFAOYSA-N	7.0	(*21*)
2-methyl-1,2-oxazolidin-3-one	CN1OCCC1=O	DGVORXWMCNREFA-UHFFFAOYSA-N	7.0	(*10*)
1-chloro-n,n-diethylacetamide	CCN(CC)C(=O)CCl	CQQUWTMMFMJEFE-UHFFFAOYSA-N	7.0	(*21*)
n,n-diphenylbutanamide	CCCC(=O)N(c1ccccc1)c1ccccc1	UKROGNGFIXLRHI-UHFFFAOYSA-N	7.1	(*21*)
1-phenyl-2-pyrrolidinone	O=C1CCCN1c1ccccc1	JMVIVASFFKKFQK-UHFFFAOYSA-N	7.1	(*21*)(*21*)
1-(3-methylphenyl)-2-pyrrolidinone	Cc1cccc(N2CCCC2=O)c1	XQAACMFZWHCPPN-UHFFFAOYSA-N	7.2	(*21*)
n,n-diphenylacetamide	CC(=O)N(c1ccccc1)c1ccccc1	DKLYDESVXZKCFI-UHFFFAOYSA-N	7.2,7.4	(*21*)(*31*)
1-(4-methylphenyl)-2-pyrrolidinone	Cc1ccc(N2CCCC2=O)cc1	ORPHOKOVVUFNKE-UHFFFAOYSA-N	7.3	(*21*)
1-(4-ethylphenyl)-2-pyrrolidinone	CCc1ccc(N2CCCC2=O)cc1	SAANJXKHPZBABZ-UHFFFAOYSA-N	7.3	(*21*)

Common Name	**Canonical Smiles**	**InChIKey**	β	**References**
n,n-dimethyl-4-nitrobenzamide	CN(C)C(=O)c1ccc([N+](=O)[O-])cc1S(N)(=O)=O	WYOXDERVKORKJN-UHFFFAOYSA-N	7.3	(*31*)
n,n-dimethyl-4-(trifluoromethyl)ben zamide	CN(C)C(=O)c1ccc(C(F)(F)F)cc1	NOFXHGGTQGRTTJ-UHFFFAOYSA-N	7.4	(*31*)
methylimidoformic acid	CNC=O	ATHHXGZTWNVVOU-UHFFFAOYSA-N	7.4	(*31*)(*20*)
n,n-dimethylformamide	CN(C)C=O	ZMXDDKWLCZADIW-UHFFFAOYSA-N	7.4,7.7	(*21*)(*31*)
1-(4-methoxyphenyl)-2-pyrrolidinone	COc1ccc(N2CCCC2=O)cc1	IDJCCRRYIMWLSQ-UHFFFAOYSA-N	7.5	(*21*)
n,n-diethylformamide	CCN(C=O)CC	SUAKHGWARZSWIH-UHFFFAOYSA-N	7.5,7.7	(*21*)(*31*)
n,n-dicyclohexyl-2,2-dimethylpropio namide	CC(C)(C)C(=O)N(C1CCCCC1)C1CCCCC1	DQWXPGSGBJVHPN-UHFFFAOYSA-N	7.6	(*31*)
n-methylbenzamide	CNC(=O)c1ccccc1	NCCHARWOCKOHIH-UHFFFAOYSA-N	7.6	(*31*)
n,n tert-butyl methyl tert butylamide	CN(C(=O)C(C)(C)C)C(C)(C)C	JNAKRDAEBSBJGO-UHFFFAOYSA-N	7.6	(*10*)
n,n-diisopropyl-2,2-dimethylpropion amide	CC(C)N(C(=O)C(C)(C)C)C(C)C	WBDSPWDNJYQQDT-UHFFFAOYSA-N	7.6	(*31*)
n,n-dimethylbenzamide	CN(C)C(=O)c1ccccc1	IMNDHOCGZLYMRO-UHFFFAOYSA-N	7.6,8.0	(*21*)(*31*)
n,n-dimethyl-4-bromobenzamide	CN(C)C(=O)c1ccc(Br)cc1	BRRVYBRXLUEEJP-UHFFFAOYSA-N	7.7	(*31*)
n,n-diethylpropanamide	CCC(=O)N(CC)CC	YKOQQFDCCBKROY-UHFFFAOYSA-N	7.7	(*21*)
1-formylpiperidine	O=CN1CCCCC1	FEWLNYSYJNLUOO-UHFFFAOYSA-N	7.7	(*31*)
n-(2-chlorophenyl)pyrrolidin-2-one	O=C1CCCN1c1ccccc1Cl	UCCTWLQOBSQILV-UHFFFAOYSA-N	7.8	(*21*)
n,n-dimethyl-4-fluorobenzamide	CN(C)C(=O)c1ccc(F)cc1	NUOGEPIJFRZXIN-UHFFFAOYSA-N	7.8	(*31*)
n,n,2,2-tetramethylpropanamide	CN(C)C(=O)C(C)(C)C	RLVGHTRVYWUWSH-UHFFFAOYSA-N	7.8,7.7	(*21*)(*31*)
n,n-diethylbenzamide	CCN(CC)C(=O)c1ccccc1	JLNGEXDJAQASHD-UHFFFAOYSA-N	7.8,8.0	(*21*)(*31*)
phenyl(1-piperidinyl)methanone	O=C(c1ccccc1)N1CCCCC1	YXTROGRGRSPWKL-UHFFFAOYSA-N	7.9	(*21*)
n,n-diethyldecanamide	CCCCCCCCCC(=O)N(CC)CC	OOYRLFIIUVBZSY-UHFFFAOYSA-N	7.9	(*21*)
n-methylacetanilide	CC(=O)N(C)c1ccccc1	LMTGCJANOQOGPI-UHFFFAOYSA-N	7.9	(*31*)
n,n-dimethylsobutylamide	CC(C)CC(=O)N(C)C	LVQDLURAEDSMES-UHFFFAOYSA-N	7.9	(*21*)
n,n-diethylnicotinamide	CCN(CC)C(=O)c1cccnc1	NCYVXEGFNDZQCU-UHFFFAOYSA-N	7.9,7.7	(*21*)(*10*)
n,n-diethylbutanamide	CCCC(=O)N(CC)CC	CDQSTBHGKNNPSY-UHFFFAOYSA-N	7.9	(*21*)(*21*)
n,n-dimethylpropanamide	CCC(=O)N(C)C	MBHINSULENHCMF-UHFFFAOYSA-N	7.9,8.3	(*21*)(*31*)
n,n-dicyclohexyl-2-methylpropanamide	CC(C)C(=O)N(C1CCCCC1)C1CCCCC1	BUFHMXOHXTZRDH-UHFFFAOYSA-N	8.0	(*31*)
n-methylpropionamide	CCC(=O)NC	QJQAMHYHNCADNR-UHFFFAOYSA-N	8.0	(*31*)
n-propionylpiperidine	CCC(=O)N1CCCCC1	MTJVUMGKHCIMJL-UHFFFAOYSA-N	8.0	(*21*)
n-butyrylpiperidine	CCCC(=O)N1CCCCC1	QANVSPFERJBPTO-UHFFFAOYSA-N	8.0	(*21*)
n,n-dicyclohexylbenzamide	O=C(c1ccccc1)N(C1CCCCC1)C1CCCCC1	QJUBWCXHSCFIHV-UHFFFAOYSA-N	8.0	(*21*)
n,n-dicyclohexylpropanamide	CCC(=O)N(C1CCCCC1)C1CCCCC1	HUTDHWXNOSDRBN-UHFFFAOYSA-N	8.0	(*21*)(*31*)

Common Name	Canonical Smiles	InChIKey	β	References
(1z)-n-methylethanimidic acid	CNC(C)=O	OHLUUHNLEMFGTQ-UHFFFAOYSA-N	8.0,8.1,8.2	(*21*)(*31*)(*20*)
1-(2-methoxyphenyl)-2-pyrrolidinone	COc1ccccc1N1CCCC1=O	SMBILOIZRKUZPE-UHFFFAOYSA-N	8.1	(*21*)
n-ethylacetamide	CCNC(C)=O	PMDCZENCAXMSOU-UHFFFAOYSA-N	8.1	(*31*)
n,n-dimethyl-4-methylbenzamide	Cc1ccc(C(=O)N(C)C)cc1	ULKWBVNMJZUEBD-UHFFFAOYSA-N	8.1	(*31*)
n,n,2-trimethylpropanamide	CC(C)C(=O)N(C)C	GXMIHVHJTLPVKL-UHFFFAOYSA-N	8.1	(*21*)(*31*)
n,n-diethylacetamide	CCN(CC)C(C)=O	AJFDBNQQDYLMJN-UHFFFAOYSA-N	8.1,8.5	(*21*)(*21*)(*31*)
n,n-dimethylacetamide	CC(=O)N(C)C	FXHOOIRPVKKKFG-UHFFFAOYSA-N	8.1,8.5	(*21*)(*31*)(*20*)
n,n-dimethyl-4-methoxybenzamide	COc1ccc(C(=O)N(C)C)cc1	OCGXPFSUJVHRHA-UHFFFAOYSA-N	8.2	(*31*)
n-acetylpiperidine	CC(=O)N1CCCCC1	KDISMIMTGUMORD-UHFFFAOYSA-N	8.2	(*21*)
n,n-diethyl-4-methoxybenzamide	CCN(CC)C(=O)c1ccc(OC)cc1	HCJXEOFLVIFFDG-UHFFFAOYSA-N	8.3	(*31*)
1-methyl-2-pyrrolidinone	CN1CCCC1=O	SECXISVLQFMRJM-UHFFFAOYSA-N	8.5,8.3	(*21*)(*31*)
n,n-dicyclohexylacetamide	CC(=O)N(C1CCCCC1)C1CCCCC1	KYVIFDXEMABEDB-UHFFFAOYSA-N	8.5,8.4	(*21*)(*31*)
n,n-dimethyl-4-dimethylaminobenzamide	CN(C)C(=O)c1ccc(N(C)C)cc1	SWIMPUZQSVMCCL-UHFFFAOYSA-N	8.6	(*31*)
n-methylcaprolactam	CN1CCCCCC1=O	ZWXPDGCFMMFNRW-UHFFFAOYSA-N	8.7	(*31*)
1-methyl-2-piperidone	CN1CCCCC1=O	GGYVTHJIUNGKFZ-UHFFFAOYSA-N	8.8	(*31*)
pyrrolidin-2-one	O=C1CCCN1	HNJBEVLQSNELDL-UHFFFAOYSA-N	8.9	(*21*)
n,n-diethylisonicotinamide	CCN(CC)C(=O)c1ccncc1	CDQAJSRQKGFYDY-UHFFFAOYSA-N	10.9	

3.4.16 PYRIDONE

Common Name	Canonical Smiles	InChIKey	β	References
1,3-dimethyluracil	Cn1ccc(=O)n(C)c1=O	JSDBKAHWADVXFU-UHFFFAOYSA-N	7.0	(*21*)
3-methyl-4-pyrimidone	Cn1cnccc1=O	PSXLJUKMMIHADB-UHFFFAOYSA-N	7.2	(*21*)
1-methyl-2(1h)-pyridinone	Cn1ccccc1=O	DVVGIUUJYPYENY-UHFFFAOYSA-N	8.5,8.8	(*21*)(*31*)(*20*)

3.4.17 ACETYL FLUORIDE

Common Name	Canonical Smiles	InChIKey	β	References
benzoyl fluoride	O=C(F)c1ccccc1	HPMLGNIUXVXALD-UHFFFAOYSA-N	2.4	(*21*)
propionyl fluoride	CCC(=O)F	WMFABESKCHGSRC-UHFFFAOYSA-N	2.8	(*21*)

3.4.18 CARBONATE

Common Name	Canonical Smiles	InChIKey	β	References
vinylene carbonate	O=c1occo1	VAYTZRYEBVHVLE-UHFFFAOYSA-N	4.6	(*29*)
dimethyl carbonate	COC(=O)OC	IEJIGPNLZYLLBP-UHFFFAOYSA-N	4.9	(*29*)
ethyl methyl carbonate	CCOC(=O)OC	JBTWLSYIZRCDFO-UHFFFAOYSA-N	4.9	(*29*)
diethyl carbonate	CCOC(=O)OCC	OIFBSDVPJOWBCH-UHFFFAOYSA-N	5.0	(*29*)(*20*)
4-methyl-1,3-dioxolan-2-one	C[C@H]1COC(=O)O1	RUOJZAUFBMNUDX-VKHMYHEASA-N	5.8	(*29*)

3.4.19 THIOCARBONATE

Common Name	Canonical Smiles	InChIKey	β	References
s-ethyl methylcarbonate	CCSC(=O)OC	VVIAWLIDZAXESO-UHFFFAOYSA-N	4.7	(*29*)

3.4.20 UREA

Common Name	Canonical Smiles	InChIKey	β	References
1,1,3,3-tetraphenylurea	O=C(N(c1ccccc1)c1ccccc1)N(c1ccccc1)c1ccccc1	ZVWHURINXJWEER-UHFFFAOYSA-N	6.9	(*31*)
1,1-diphenyl-3,3-diethylurea	CCN(CC)C(=O)N(c1ccccc1)c1ccccc1	DQYDFMBXYUTXOK-UHFFFAOYSA-N	7.7	(*31*)
1,1-diphenyl-3,3-dimethylurea	CN(C)C(=O)N(c1ccccc1)c1ccccc1	JPMQWSJHCDLANT-UHFFFAOYSA-N	7.7	(*31*)
1,3-diphenyl-1,3-diethylurea	CCN(C(=O)N(CC)c1ccccc1)c1ccccc1	PZIMIYVOZBTARW-UHFFFAOYSA-N	7.9	(*31*)
1,1,3,3-tetramethylurea	CN(C)C(=O)N(C)C	AVQQQNCBBIEMEU-UHFFFAOYSA-N	8.3,8.5	(*21*)(*31*)(*20*)
n,n'-dimethyl n,n'-ethyleneurea	CN1CCN(C)C1=O	CYSGHNMQYZDMIA-UHFFFAOYSA-N	8.5	(*31*)
1,1,3,3-tetraethylurea	CCN(CC)C(=O)N(CC)CC	UWHSPZZUAYSGTB-UHFFFAOYSA-N	8.5	(*31*)
1,3-dimethyltetrahydro-2(1h)-pyrimidinone	CN1CCCN(C)C1=O	GUVUOGQBMYCBQP-UHFFFAOYSA-N	9.3	(*31*)

3.4.21 ACETAMIDATE

Common Name	Canonical Smiles	InChIKey	β	References
me3[n+][n-]c(=o)p-cf3c6h5	C[N+](C)(C)[N-]C(=O)c1ccc(C(F)(F)F)cc1	AXDJVNWJCWMTJY-UHFFFAOYSA-N	8.8	(*32*)
n-trimethylammonio-p-methoxybenzamidate	COc1ccc(C(=O)[N-][N+](C)(C)C)cc1	QKUTVFWSNXJWFO-UHFFFAOYSA-N	9.6	(*32*)
me3[n+][n-]c(=o)nonyl	CCCCCCCCCC(=O)[N-][N+](C)(C)C	FMCZKECPZDBHQL-UHFFFAOYSA-N	10.4	(*32*)
me3[n+][n-]c(=o)tbu	CC(C)(C)C(=O)[N-][N+](C)(C)C	QFDOXTPAGKPVEV-UHFFFAOYSA-N	10.4	(*32*)
me3[n+][n-]c(=o)1-adamantyl	C[N+](C)(C)[N-]C(=O)C12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3	RLYBUPBSBHBSJ-VNHJDHJASA-N	10.5	(*32*)
n-trimethylammonioacetamidate	CC(=O)[N-][N+](C)(C)C	IUFAEQDMEMKFCW-UHFFFAOYSA-N	10.6	(*32*)
me3[n+][n-]c(=o)ipr	CC(C)C(=O)[N-][N+](C)(C)C	WMNKYPLFYPNCSX-UHFFFAOYSA-N	10.7	(*32*)
me3[n+][n-]c(=o)et	CCC(=O)[N-][N+]C(C)(C)C	QSEQJBQZMRTPHG-UHFFFAOYSA-N	10.9	(*32*)

3.4.22 CARBAMATE

Common Name	Canonical Smiles	InChIKey	β	References
phenyl diphenylcarbamate	O=C(Oc1ccccc1)N(c1ccccc1)c1ccccc1	XSJJNRDFIMCZRS-UHFFFAOYSA-N	5.7	(*31*)
methyl diphenylcarbamate	COC(=O)N(c1ccccc1)c1ccccc1	SYMPSOJKDIMXKZ-UHFFFAOYSA-N	6.2	(*31*)
ethyl diphenylcarbamate	CCOC(=O)N(c1ccccc1)c1ccccc1	HKTSLDUAGCAISP-UHFFFAOYSA-N	6.3	(*31*)
phenyl dimethylcarbamate	CN(C)C(=O)Oc1ccccc1	MYOHNZJKOAODMX-UHFFFAOYSA-N	6.8	(*31*)(*10*)
methyl dimethylcarbamate	COC(=O)N(C)C	SELYJABLPLKXOY-UHFFFAOYSA-N	7.1	(*31*)
ethyl dimethylcarbamate	CCOC(=O)N(C)C	SUDHEDJJFGYYPL-UHFFFAOYSA-N	7.1	(*31*)
ethyl diethylcarbamate	CCOC(=O)N(CC)CC	VAJCYQHLYBTSHG-UHFFFAOYSA-N	7.4	(*31*)

3.4.23 CARBAMOYL CHLORIDE

Common Name	Canonical Smiles	InChIKey	β	References
diphenylcarbamoyl chloride	O=C(Cl)N(c1ccccc1)c1ccccc1	XNBKKRFABABBPM-UHFFFAOYSA-N	4.7	(*31*)
dimethylcarbomyl chloride	CN(C)C(=O)Cl	YIIMEMSDCNDGTB-UHFFFAOYSA-N	5.3	(*31*)
diethylcarbamoyl chloride	CCN(CC)C(=O)Cl	OFCCYDUUBNUJIB-UHFFFAOYSA-N	5.5	(*31*)

3.4.24 THIOESTER

Common Name	Canonical Smiles	InChIKey	β	References
dihydro-2(3h)-thiophenone	O=C1CCCS1	KMSNYNIWEORQDJ-UHFFFAOYSA-N	5.2	(*10*)

3.4.25 N-NITROSO

Common Name	Canonical Smiles	InChIKey	β	References
n-nitroso-n-phenylaniline	O=NN(c1ccccc1)c1ccccc1	UBUCNCOMADRQHX-UHFFFAOYSA-N	4.3	(*21*)(*21*)
n-methyl-n-nitrosomethanamine	CN(C)N=O	UMFJAHHVKNCGLG-UHFFFAOYSA-N	5.8	(*21*)(*21*)

3.4.26 NITRO

Common Name	Canonical Smiles	InChIKey	β	References
3-chloronitrobenzene	O=[N+]([O-])c1cccc(Cl)c1	KMAQZIILEGKYQZ-UHFFFAOYSA-N	3.4	(*33*)
4-chloronitrobenzene	O=[N+]([O-])c1ccc(Cl)cc1	CZGCEKJOLUNIFY-UHFFFAOYSA-N	3.6	(*33*)
nitromethane	C[N+](=O)[O-]	LYGJENNIWJXYER-UHFFFAOYSA-N	3.7	(*33*)(*20*)
4-nitrophenyl acetate	COC(=O)c1ccc([N+](=O)[O-])cc1	YOJAHJGBFDPSDI-UHFFFAOYSA-N	3.8	(*29*)
4-nitrotoluene	Cc1ccc([N+](=O)[O-])cc1	ZPTVNYMJQHSSEA-UHFFFAOYSA-N	3.8	(*33*)
4-nitrophenyl acetate	CC(=O)Oc1ccc([N+](=O)[O-])cc1	QAUUDNIGJSLPSX-UHFFFAOYSA-N	3.8	(*29*)
nitroethane	CC[N+](=O)[O-]	MCSAJNNLRCFZED-UHFFFAOYSA-N	3.8	(*33*)
4-nitrobenzaldehyde	O=Cc1ccc([N+](=O)[O-])cc1	BXRFQSNOROATLV-UHFFFAOYSA-N	3.9	(*21*)
2-methyl-2-nitropropane	CC(C)(C)[N+](=O)[O-]	AIMREYQYBFBEGQ-UHFFFAOYSA-N	4.0	(*33*)
2-nitropropane	CC(C)[N+](=O)[O-]	FGLBSLMDCBOPQK-UHFFFAOYSA-N	4.0	(*33*)
1,2-dimethyl-4-nitrobenzene	Cc1ccc([N+](=O)[O-])cc1C	HFZKOYWDLDYELC-UHFFFAOYSA-N	4.1	(*33*)
nitrobenzene	O=[N+]([O-])c1ccccc1	LQNUZADURLCDLV-UHFFFAOYSA-N	4.1,3.7	(*21*)(*33*)
4-nitroanisole	COc1ccc([N+](=O)[O-])cc1	BNUHAJGCKIQFGE-UHFFFAOYSA-N	4.2	(*33*)
ethyl 4-nitrobenzoate	CCOC(=O)c1ccc([N+](=O)[O-])cc1	PHWSCBWNPZDYRI-UHFFFAOYSA-N	4.5	(*29*)
1-(4-nitrophenyl)ethanone	CC(=O)c1ccc([N+](=O)[O-])cc1	YQYGPGKTNQNXMH-UHFFFAOYSA-N	4.6	(*30*)
n,n-diethyl-4-nitroaniline	CCN(CC)c1ccc([N+](=O)[O-])cc1	CFPIZMWTMRWZRO-UHFFFAOYSA-N	5.1	(*33*)
(e)-n,n-dimethyl-2-nitroethenamine	CN(C)/C=C/[N+](=O)[O-]	JKOVQYWMFZTKMX-ONEGZZNKSA-N	6.3,6.6	(*33*)(*20*)
1-(2-nitrovinyl)piperidine	O=[N+]([O-])/C=C/N1CCCCC1	IGTWYMQBGKAFCF-VOTSOKGWSA-N	6.5	(*33*)

3.4.27 NITROAMINE

Common Name	Canonical Smiles	InChIKey	β	References
(1r,2e,4r)-1,7,7-trimethyl-n-nitrob icyclo[2.2.1]heptan-2-imine	CC1(C)[C@@H]2CC[C@@]1(C)/C(=N/[N+](=O)[O-])C2	QWPYVYJPIHGYGX-RZIOALPKSA-N	3.8	(*33*)

3.4.28 N-OXIDE

Common Name	Canonical Smiles	InChIKey	β	References
pyridine N-oxide	[O-][n+]1ccccc1	ILVXOBCQQYKLDS-UHFFFAOYSA-N	9.0,9.1	(*21*)(*20*)
trimethylamine N-oxide	C[N+](C)(C)[O-]	UYPYRKYUKCHHIB-UHFFFAOYSA-N	13.1	(*34*)

3.4.29 PHOSPHINE OXIDE

Common Name	Canonical Smiles	InChIKey	β	References
triphenylphosphine oxide	O=P(c1ccccc1)(c1ccccc1)c1ccccc1	FIQMHBFVRAXMOP-UHFFFAOYSA-N	10.1	(*21*)
tributylphosphine oxide	CCCCP(=O)(CCCC)CCCC	MNZAKDODWSQONA-UHFFFAOYSA-N	10.2, 10.7	(*21*)(*35*)
trimethylphosphine oxide	CP(C)(C)=O	LRMLWYXJORUTBG-UHFFFAOYSA-N	10.7	(*21*)
tripropylphosphine oxide	CCCP(=O)(CCC)CCC	SNZSAFILJOCMFM-UHFFFAOYSA-N	10.8	(*21*)
triethylphosphine oxide	CCP(=O)(CC)CC	ZSSWXNPRLJLCDU-UHFFFAOYSA-N	11.1,10.1	(*21*)(*20*)

3.4.30 PHOSPHATE

Common Name	Canonical Smiles	InChIKey	β	References
triphenyl phosphate	O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1	XZZNDPSIHUTMOC-UHFFFAOYSA-N	7.0	(*21*)
5,5-dimethyl-2-phenoxy-1,3,2-dioxaphosphinane 2-oxide	CC1(C)COP(=O)(Oc2ccccc2)OC1	VSKVZTVOVPEFOH-UHFFFAOYSA-N	7.3	(*36*)
trimethyl phosphate	COP(=O)(OC)OC	WVLBCYQITXONBZ-UHFFFAOYSA-N	8.5	(*21*)
tributyl phosphate	CCCCOP(=O)(OCCCC)OCCCC	STCOOQWBFONSKY-UHFFFAOYSA-N	8.6	(*21*)
triethyl phosphate	CCOP(=O)(OCC)OCC	DQWPFSLDHJDLRL-UHFFFAOYSA-N	8.8	(*21*)

3.4.31 PHOSPHITE

Common Name	Canonical Smiles	InChIKey	β	References
dimethyl phosphite	CO[PH](=O)OC	HZCDANOFLILNSA-UHFFFAOYSA-N	8.0	(*21*)
diethyl phosphite	CCO[PH](=O)OCC	MJUJXFBTEFXVKU-UHFFFAOYSA-N	8.3	(*21*)
diisopropyl phosphite	CC(C)O[PH](=O)OC(C)C	BLKXLEPPVDUHBY-UHFFFAOYSA-N	8.6	(*21*)

3.4.32 PHOSPHONIC ACID

Common Name	Canonical Smiles	InChIKey	β	References
5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide	CC1(C)CO[PH](=O)OC1	QHXZLTUNAVKFIT-UHFFFAOYSA-N	7.2	(*36*)

3.4.33 PHOSPHONATE

Common Name	Canonical Smiles	InChIKey	β	References
3,2-dioxaphosphinane 2-oxide	CC1(C)COP(=O)(C(Cl)(Cl)Cl)OC1	CGMXYGZTTKIENK-UHFFFAOYSA-N	6.6	(*36*)
diethyl trichloromethylphosphonate	CCOP(=O)(OCC)C(Cl)(Cl)Cl	RVAQSYWDOSHWGP-UHFFFAOYSA-N	7.3	(*21*)
diethyl dichloromethylphosphonate	CCOP(=O)(OCC)C(Cl)Cl	XDOKVFJJVSLHDJ-UHFFFAOYSA-N	7.8	(*21*)
2-methoxy-5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide	COP1(=O)OCC(C)(C)CO1	HHZSLQGPHYVMOQ-UHFFFAOYSA-N	7.8	(*36*)
5,5-dimethyl-2-phenyl-1,3,2-dioxaphosphinane 2-oxide	CC1(C)COP(=O)(c2ccccc2)OC1	IBGSBHZFACCHSP-UHFFFAOYSA-N	8.4	(*36*)
diethyl (chloromethyl)phosphonate	CCOP(=O)(CCl)OCC	MZBIWKMCTWJLPT-UHFFFAOYSA-N	8.5	(*21*)
diethyl tritylphosphonate	CCOP(=O)(OCC)C(c1ccccc1)(c1ccccc1)c1ccccc1	AEMDEBJSSOOMNM-UHFFFAOYSA-N	8.6	(*36*)
2,5,5-trimethyl-1,3,2-dioxaphosphinane 2-oxide	CC1(C)COP(C)(=O)OC1	PQSCITIRWCGOKJ-UHFFFAOYSA-N	8.6	(*36*)
2-benzyl-5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide	CC1(C)COP(=O)(Cc2ccccc2)OC1	QULASSAQFUJMIP-UHFFFAOYSA-N	8.6	(*36*)
di-(1-chloropropyl) methylphosphonate	CC[C@H](Cl)O[P@](C)(=O)O[C@H](Cl)CC	IWJMFKRJGSKMBW-SHRKTGAESA-N	8.7	(*21*)
dimethyl ethylphosphonate	CCP(=O)(OC)OC	YHQMSHVVGOSZEW-UHFFFAOYSA-N	9.0	(*21*)
dimethyl methylphosphonate	COP(C)(=O)OC	VONWDASPFIQPDY-UHFFFAOYSA-N	9.1	(*37*)
5,5-dimethyl-2-(trichloromethyl)-1, diethyl methylphosphonate	CCOP(C)(=O)OCC	NYYLZXREFNYPKB-UHFFFAOYSA-N	9.1	(*21*)
diethyl isopropylphosphonate	CCOP(=O)(OCC)C(C)C	PPMDSXRMQXBCJW-UHFFFAOYSA-N	9.1	(*21*)
diethyl ethylphosphonate	CCOP(=O)(CC)OCC	AATNZNJRDOVKDD-UHFFFAOYSA-N	9.2	(*21*)

3.4.34 OTHER P=O

Common Name	Canonical Smiles	InChIKey	β	References
heptyne	C#CCCCCC	YVXHZKKCZYLQOP-UHFFFAOYSA-N	3.0	(*11*)
o-prop-2-ynyl bis(dimethylamino)thi ophosphinate	C#CCOP(=S)(N(C)C)N(C)C	HDWKOGROOOQOOX-UHFFFAOYSA-N	5.1	(*11*)
3-propynyl phosphorodichloridate	C#CCOP(=O)(Cl)Cl	XHEYZHCJHWNLAA-UHFFFAOYSA-N	5.2	(*11*)
2-chloro-5,5-dimethyl-1,3,2-dioxaph osphinane 2-oxide	CC1(C)COP(=O)(Cl)OC1	VZMUCIBBVMLEKC-UHFFFAOYSA-N	6.4	(*36*)
o,o-diethyl s-methylâ phosphorothioate	CCOP(=O)(OCC)SC	GWEDODYYNURODY-UHFFFAOYSA-N	7.8	(*36*)
n,n,n',n'-tetramethylphosphorodiami dic chloride	CN(C)P(=O)(Cl)N(C)C	WYLQARGYFXBZMD-UHFFFAOYSA-N	8.5	(*11*)
s-prop-2-ynyl bis(dimethylamino)thi ophosphinate	C#CCSP(=O)(N(C)C)N(C)C	JEFWAOURROPQAD-UHFFFAOYSA-N	8.9	(*11*)
diethyl diethylphosphoramidate	CCOP(=O)(OCC)N(CC)CC	SZAAJLKHJPJRJQ-UHFFFAOYSA-N	9.0	(*36*)
prop-2-ynyl bis(morpholino)phosphin ate	C#CCOP(=O)(N1CCOCC1)N1CCOCC1	ZWZFGONTTYIELP-UHFFFAOYSA-N	9.0	(*11*)
1-[aziridin-1-yl(prop-2-ynoxy)phosp horyl]aziridine	C#CCOP(=O)(N1CC1)N1CC1	DMGBLQXOZQWUAR-UHFFFAOYSA-N	9.0	(*11*)
N/A	C#CCN(CC)P(=O)(N(C)C)N(C)C	DETZZVPMDQPJIC-UHFFFAOYSA-N	9.3	(*11*)
prop-2-ynyl bis(dibutylamino)phosph inate	C#CCOP(=O)(N(CCCC)CCCC)N(CCCC)CCCC	UIZVATMSLGDSAW-UHFFFAOYSA-N	9.4	(*11*)
but-3-ynyl bis(dimethylamino)phosph inate	C#CCCOP(=O)(N(C)C)N(C)C	GYHSJCJMDZRRJG-UHFFFAOYSA-N	9.5	(*11*)
prop-2-ynyl bis(dimethylamino)phosp hinate	C#CCOP(=O)(N(C)C)N(C)C	MFXVLTAAMOAZMS-UHFFFAOYSA-N	9.6	(*11*)
prop-2-ynyl bis(diethylamino)phosph inate	C#CCOP(=O)(N(CC)CC)N(CC)CC	DEHSPEZTBSYMPL-UHFFFAOYSA-N	9.7	(*11*)
prop-2-ynyl bis(piperidino)phosphinate	C#CCOP(=O)(N1CCCCC1)N1CCCCC1	RVDBZQDTMHPUAJ-UHFFFAOYSA-N (	10.1	(*11*)
n-methyl n-propargyl bis-dimethylph osphoramide	C#CCN(C)P(=O)(N(C)C)N(C)C	DOYODMYEMDHHCE-UHFFFAOYSA-N	10.4	(*11*)
HMPA	CN(C)P(=O)(N(C)C)N(C)C	GNOIPBMMFNIUFM-UHFFFAOYSA-N	10.8,10.9,11.0	(*11*)(*21*)(*20*)

3.4.35 SULFOXIDE

Common Name	Canonical Smiles	InChIKey	β	References
1,1'-sulfinyldibenzene	O=S(c1ccccc1)c1ccccc1	JJHHIJFTHRNPIK-UHFFFAOYSA-N	7.5	(*21*)(*21*)
(methylsulfinyl)benzene	C[S@](=O)c1ccccc1	JXTGICXCHWMCPM-VIFPVBQESA-N	7.8	(*21*)
1,1'-sulfinylbis(4-methylbenzene)	Cc1ccc(S(=O)c2ccc(C)cc2)cc1	MJWNJEJCQHNDNM-UHFFFAOYSA-N	7.8	(*21*)
tetrahydrothiophene s-oxide	O=S1CCCC1	ISXOBTBCNRIIQO-UHFFFAOYSA-N	8.6	(*21*)
DMSO	CS(C)=O	IAZDPXIOMUYVGZ-UHFFFAOYSA-N	8.6,8.8	(*21*)(*20*)
dibutyl sulphoxide	CCCCS(=O)CCCC	LOWMYOWHQMKBTM-UHFFFAOYSA-N	8.7	(*21*)
di-isopropyl sulphoxide	CC(C)S(=O)C(C)C	WFJXYIUAMJAURQ-UHFFFAOYSA-N	8.7	(*21*)

3.4.36 SULFONE

Common Name	Canonical Smiles	InChIKey	β	References
diphenyl sulphone	O=S(=O)(c1ccccc1)c1ccccc1	KZTYYGOKRVBIMI-UHFFFAOYSA-N	5.9,5.8	(*21*)(*38*)
tetrahydrothiopheneâ 1,1-dioxide	O=S1(=O)CCCC1	HXJUTPCZVOIRIF-UHFFFAOYSA-N	6.0,6.3	(*21*)(*38*)
dimethyl sulphone	CS(C)(=O)=O	HHVIBTZHLRERCL-UHFFFAOYSA-N	6.2	(*38*)
dibutyl sulphone	CCCCS(=O)(=O)CCCC	AIDFJGKWTOULTC-UHFFFAOYSA-N	6.4	(*38*)

3.4.37 SULFITE

Common Name	Canonical Smiles	InChIKey	β	References
diethyl sulphite	CCOS(=O)OCC	NVJBFARDFTXOTO-UHFFFAOYSA-N	4.9	(*21*)

3.4.38 SULFATE

Common Name	Canonical Smiles	InChIKey	β	References
diethyl sulphate	CCOS(=O)(=O)OCC	DENRZWYUOJLTMF-UHFFFAOYSA-N	4.8	(*38*)(*20*)

3.4.39 SULFONATE

Common Name	Canonical Smiles	InChIKey	β	References
ethyl methanesulfonate	CCOS(C)(=O)=O	PLUBXMRUUVWRLT-UHFFFAOYSA-N	5.3	(*38*)

3.4.40 SULFAMIDE

Common Name	Canonical Smiles	InChIKey	β	References
n,n,n',n'-tetraethylsulfamide	CCN(CC)S(=O)(=O)N(CC)CC	IYIAWAACGTUPCC-UHFFFAOYSA-N	6.3	(*38*)

3.4.41 SULFINAMIDE

Common Name	Canonical Smiles	InChIKey	β	References
n,n-dimethylbenzenesulfinamide	CN(C)[S@](=O)c1ccccc1	HLDBHWJNZHGZMV-LLVKDONJSA-N	7.6	(*21*)
n,n-dimethyltoluene-p-sulphonamide	Cc1ccc([S@](=O)N(C)C)cc1	NPZOFLLFFNIYON-LBPRGKRZSA-N	7.7	(*21*)
n,n-dimethylmethanesulfinamide	CN(C)[S@](C)=O	AQNQZLOSBFEYBX-LURJTMIESA-N	8.2	(*21*)(*21*)

3.4.42 SULFONAMIDE

Common Name	Canonical Smiles	InChIKey	β	References
2-benzyl-1,2-benzothiazol-3(2h)-one 1,1-dioxide	O=C1c2ccccc2S(=O)(=O)N1Cc1ccccc1	JLGPMOJYECOCEP-UHFFFAOYSA-N	4.6	(*10*)
n-benzyl-n-methylbenzenesulfonamide	CN(Cc1ccccc1)S(=O)(=O)c1ccccc1	NMRHCNYNTKGDGB-UHFFFAOYSA-N	5.2	(*10*)
n-methylmethanesulfonamide	CNS(C)(=O)=O	UHNHTTIUNATJKL-UHFFFAOYSA-N	5.9	(*21*)
n,n-dimethylmethanesulfonamide	CN(C)S(C)(=O)=O	WCFDSGHAIGTEKL-UHFFFAOYSA-N	5.9,6.0	(*21*)(*38*)
n,n-dimethylbenzenesulfonamide	CN(C)S(=O)(=O)c1ccccc1	BVSPJPNNLDIUFE-UHFFFAOYSA-N	6.1,5.7	(*21*)(*38*)(*20*)
n,n-dimethyltoluene-p-sulphonamide	Cc1ccc([S@@](=O)(O)N(C)C)cc1	LPZKWQRDFJJRDI-UHFFFAOYSA-N	6.2	(*21*)
n-[(dimethylamino)methylene]benzene sulfonamide	CN(C)/C=N/S(=O)(=O)c1ccccc1	WDGYPUOJGIEZMO-CSKARUKUSA-N	7.1	(*38*)
n,n,4-trimethylbenzenesulfonamide	Cc1ccc(S(=O)(=O)N(C)C)cc1	WZKOKGOAHBIPCI-UHFFFAOYSA-N	7.7	(*21*)
n-(dimethyl-lambda 4 -sulfanylidene)-4-methylbenzenesulfonamide	Cc1ccc(S(=O)(=O)N=S(C)C)cc1	XXOIGDFCELVFFJ-UHFFFAOYSA-N	7.8	(*38*)
2,2,2-trimethyl-1-[(4-methylphenyl) sulfonyl]diazan-2-ium-1-ide	Cc1ccc(S(=O)(=O)[N-][N+](C) (C)C)cc1	DXVVZIGSMCTRDV-UHFFFAOYSA-N	8.9	(*38*)
2,2,2-trimethyl-1-(octylsulfonyl)di azan-2-ium-1-ide	CCCCCCCCS(=O)(=O)[N-][N+](C)(C)C	CHSPMZWZNFDUDE-UHFFFAOYSA-N	9.5	(*38*)

3.5 SULFUR

3.5.1 THIOETHER

Common Name	Canonical Smiles	InChIKey	β	References
ethyl methyl sulphide	CCSC	WXEHBUMAEPOYKP-UHFFFAOYSA-N	3.1	(*21*)
tetrahydrothiophene	C1CCSC1	RAOIDOHSFRTOEL-UHFFFAOYSA-N	3.3,3.7	(*21*)(*20*)
isobuty n-butyl sulphide	CCCCSCC(C)C	PWXRDOSRCIGJDM-UHFFFAOYSA-N	3.5	(*21*)
dimethyl sulphide	CSC	QMMFVYPAHWMCMS-UHFFFAOYSA-N	3.5	(*21*)
dibutyl sulphide	CCCCSCCCC	HTIRHQRTDBPHNZ-UHFFFAOYSA-N	3.6	(*21*)
1-(sec-butylsulfanyl)butane	CCCCS[C@@H](C)CC	JEJBXIHZMUVILV-QMMMGPOBSA-N	3.6	(*21*)
diethyl sulphide	CCSCC	LJSQFQKUNVCTIA-UHFFFAOYSA-N	3.6	(*21*)
di(tert-butyl) sulphide	CC(C)(C)SC(C)(C)C	LNMBCRKRCIMQLW-UHFFFAOYSA-N	3.6	(*21*)
tert-butyl n-butyl sulphide	CCCCSC(C)(C)C	XRYKNXGXIFPTKH-UHFFFAOYSA-N	3.7	(*21*)
diisopropyl sulphide	CC(C)SC(C)C	XYWDPYKBIRQXQS-UHFFFAOYSA-N	3.8	(*21*)

3.5.2 THIOKETONE

Common Name	Canonical Smiles	InChIKey	β	References
thiocamphor	CC1(C)[C@H]2CC[C@]1(C)C(=S)C2	AAADKYXUTOBAGS-OIBJUYFYSA-N	3.8	(*39*)

3.5.3 THIOAMIDE

Common Name	Canonical Smiles	InChIKey	β	References
n,n-dimethylthioformamide	CN(C)C=S	SKECXRFZFFAANN-UHFFFAOYSA-N	5.4	(*39*)
n,n-dimethylbenzenecarbothioamide	CN(C)C(=S)c1ccccc1	OPXCUUJACRRYMC-UHFFFAOYSA-N	5.5,5.3	(*21*)(*39*)
n,n-dimethyl-4-methoxythiobenzamide	COc1ccc(C(=S)N(C)C)cc1	DSGZADFUTPZEMZ-UHFFFAOYSA-N	5.6	(*39*)
4,n,n-trimethylthiobenzamide	Cc1ccc(C(=S)N(C)C)cc1	WZADGDPHGLPABW-UHFFFAOYSA-N	5.6	(*39*)
n-methylthioacetamide	CNC(C)=S	BNLLHLUAOXAUNQ-UHFFFAOYSA-N	5.6	(*39*)(*20*)
n,n-dimethylethanethioamide	CC(=S)N(C)C	LKNQXZAHNDFIQY-UHFFFAOYSA-N	5.7,6.0	(*21*)(*39*)
n,n-dimethyl-4-aminothiobenzamide	CN(C)C(=S)c1ccc(N)cc1	JUNNTRSMCCUKGG-UHFFFAOYSA-N	6.0	(*39*)
2-azepanethione	S=C1CCCCCN1	APLHDUWNMGJBFD-UHFFFAOYSA-N	6.6	(*39*)
2-methylpropanethioamide	CC(C)C(N)=S	NPCLRBQYESMUPD-UHFFFAOYSA-N	7.0	

3.5.4 THIOCARBAMATE

Common Name	Canonical Smiles	InChIKey	β	References
3-methyl-1,3-benzoxazole-2(3h)-thione	Cn1c(=S)oc2ccccc21	VMOIPIVQHVFUFO-UHFFFAOYSA-N	4.8	(*39*)
o-methyl dimethylcarbamothioate	COC(=S)N(C)C	QPKDBLGFWZSDSB-UHFFFAOYSA-N	4.9	(*21*)(*39*)
1,3-benzoxazole-2(3h)-thione	S=c1[nH]c2ccccc2o1	FLFWJIBUZQARMD-UHFFFAOYSA-N	5.8	(*39*)
3,4,5-trimethyl-1,3-oxazole-2(3h)-t hione	Cc1oc(=S)n(C)c1C	MQBNSGDDWSWJLR-UHFFFAOYSA-N	5.8	(*39*)
1,3-oxazolidine-2-thione	S=C1NCCO1	UMURLIQHQSKULR-UHFFFAOYSA-N	6.1	(*39*)
4,5-dimethyl-1,3-oxazole-2(3h)-thione	Cc1[nH]c(=S)oc1C	XEJIHKUDPINBCS-UHFFFAOYSA-N	7.1	(*39*)

3.5.5 DITHIOCARBAMATE

Common Name	Canonical Smiles	InChIKey	β	References
3-methyl-1,3-benzothiazole-2(3h)-th ione	Cn1c(=S)sc2ccccc21	IRNRNPNZAKHEAW-UHFFFAOYSA-N	4.5	(*39*)
methyl dimethylcarbamodithioate	CSC(=S)N(C)C	NBBZMDUHKWRYSZ-UHFFFAOYSA-N	4.7,4.5	(*21*)(*39*)
3-methyl-1,3-thiazole-2(3h)-thione	Cn1ccsc1=S	IENJMFWWRIWLIW-UHFFFAOYSA-N	4.9	(*39*)
3-methyl-1,3-thiazolidine-2-thione	CN1CCSC1=S	RGTLAJIDOSPEDH-UHFFFAOYSA-N	5.1	(*39*)
3,4,5-trimethyl-1,3-thiazole-2(3h)- thione	Cc1sc(=S)n(C)c1C	MZBUJUWHEHJJKJ-UHFFFAOYSA-N	5.6	(*39*)
1,3-benzothiazole-2(3h)-thione	S=c1[nH]c2ccccc2s1	YXIWHUQXZSMYRE-UHFFFAOYSA-N	5.6	(*39*)
1,3-thiazolidine-2-thione	S=C1NCCS1	WGJCBBASTRWVJL-UHFFFAOYSA-N	6.0	(*39*)
4,5-dimethyl-1,3-thiazole-2(3h)-thione	Cc1[nH]c(=S)sc1C	KKHBRTFQIYIHEI-UHFFFAOYSA-N	7.1	(*39*)

3.5.6 THIOUREA

Common Name	Canonical Smiles	InChIKey	β	References
1,3-dimethyl-1,3-dihydro-2h-benzimidazole-2-thione	Cn1c(=S)n(C)c2ccccc21	CSYLYUAMXUGIFE-UHFFFAOYSA-N	5.7	(*39*)
n,n-dimethyl-n',n'-diethylthiourea	CCN(CC)C(=S)N(C)C	RJSZFWIUDNOVNP-UHFFFAOYSA-N	5.9	(*39*)
1,1,3,3-tetramethylthiourea	CN(C)C(=S)N(C)C	MNOILHPDHOHILI-UHFFFAOYSA-N	5.9,6.1	(*21*)(*39*)
n,n'-dimethyl-n,n'-ethylenethiourea	CN1CCN(C)C1=S	FYHIXFCITOCVKH-UHFFFAOYSA-N	6.0	(*39*)
1-methyl-1,3-dihydro-2h-benzimidazole-2-thione	Cn1c(=S)[nH]c2ccccc21	CDNHLXOFELOEOL-UHFFFAOYSA-N	6.5	(*39*)
1,3-dimethyl-1,3-dihydro-2h-imidazole-2-thione	Cn1ccn(C)c1=S	ZYPLZLQKRFFKCL-UHFFFAOYSA-N	6.5	(*39*)
3-[(e)-(dimethylamino)methylene]-1,1-dimethylthiourea	CN(C)/C=N/C(=S)N(C)C	KBVQJEKAHKMCID-FNORWQNLSA-N	7.0	(*39*)
1,3,4,5-tetramethylimidazole-2(3h)-thione	Cc1c(C)n(C)c(=S)n1C	UEALYGMEMQDEMQ-UHFFFAOYSA-N	7.0	(*39*)
1-methyl-2-imidazolidinethione	CN1CCNC1=S	FDDDTDSPQXLQFY-UHFFFAOYSA-N	7.2	(*39*)
n-methyl-n,n'-propylenethiourea	CN1CCCNC1=S	KWRGMBARTDLYSH-UHFFFAOYSA-N	7.5	(*39*)
(1e)-n'-(dimethylcarbamothioyl)-n,n-dimethylethanimidamide	C/C(=N \C(=S)N(C)C)N(C)C	BATDBURDIROQFJ-SOFGYWHQSA-N	7.6	(*39*)
1-methyl-1h-imidazole-2-thiol	Cn1cc[nH]c1=S	PMRYVIKBURPHAH-UHFFFAOYSA-N	7.7,8.1	(*39*)(*20*)
1,4,5-trimethyl-1,3-dihydro-2h-imidazole-2-thione	Cc1[nH]c(=S)n(C)c1C	PERWAYOEWJEJNO-UHFFFAOYSA-N	7.9	(*39*)

3.5.7 ISOTHIOCYANATE

Common Name	Canonical Smiles	InChIKey	β	References
ethyl isothiocyanate	CCN=C=S	HBNYJWAFDZLWRS-UHFFFAOYSA-N	2.9	(*21*)

3.5.8 THIOCARBOYL CHLORIDE

Common Name	Canonical Smiles	InChIKey	β	References
n,n-dimethylthiocarmomyl chloride	CN(C)C(=S)Cl	PHWISQNXPLXQRU-UHFFFAOYSA-N	4.2	(*39*)

3.5.9 TRITHIOCARBONATE

Common Name	Canonical Smiles	InChIKey	β	References
ethylenetrithiocarbonate	S=C1SCCS1	XCWPBWWTGHQKDR-UHFFFAOYSA-N	3.7	(*39*)

3.5.10 THIOPHOSPHINES

Common Name	Canonical Smiles	InChIKey	β	References
o,o,o-triethyl phosphorothioate	CCOP(=S)(OCC)OCC	QTPJMTACJMLPLL-UHFFFAOYSA-N	4.7	(*21*)
hexamethylthiophosphoramide	CN(C)P(=S)(N(C)C)N(C)C	NPKXLCMBIGGTTQ-UHFFFAOYSA-N	6.0	(*21*)
tributylphosphine sulphide	CCCCP(=S)(CCCC)CCCC	FQVPFGDPYSIWTM-UHFFFAOYSA-N	6.3	(*21*)
trioctylphosphine sulphide	CCCCCCCCP(=S)(CCCCCCCC)CCCCCCCC	PIOZWDBMINZWGJ-UHFFFAOYSA-N	6.5	(*21*)

3.6 Se

3.6.1 SELENOETHER

Common Name	Canonical Smiles	InChIKey	β	References
diethyl selenide	CC[Se]CC	ALCDAWARCQFJBA-UHFFFAOYSA-N	3.4	(*21*)
dibutyl selenide	CCCC[Se]CCCC	WAULAQAPARJWJJ-UHFFFAOYSA-N	3.5	(*21*)

3.7 FLUORINE

Common Name	Canonical Smiles	InChIKey	β	References
fluorobenzene	Fc1ccccc1	PYLWMHQQBFSUBP-UHFFFAOYSA-N	1.6	(*21*)
1,3-difluoropropane	FCCCF	OOLOYCGJRJFTPM-UHFFFAOYSA-N	2.5	(*40*)
1-fluoropentane	CCCCCF	OEPRBXUJOQLYID-UHFFFAOYSA-N	2.9	(*40*)
1-fluorooctane	CCCCCCCCF	DHIVLKMGKIZOHF-UHFFFAOYSA-N	3.1	(*40*)(*20*)
fluorocyclohexane	FC1CCCCC1	GOBGVVAHHOUMDK-UHFFFAOYSA-N	3.3	(*40*)
1-fluoroadamantane	F[C@]12C[C@H]3C[C@H](C [C@H](C3)C1)C2	CPWSNJSGSXXVLD-CHIWXEEVSA-N	3.6	(*40*)

3.8 CHLORINE

Common Name	Canonical Smiles	InChIKey	β	References
tetrachloromethane	ClC(Cl)(Cl)Cl	VZGDMQKNWNREIO-UHFFFAOYSA-N	0.6	(*21*)
chloroform	ClC(Cl)Cl	HEDRZPFGACZZDS-UHFFFAOYSA-N	0.8	(*21*)
dichloromethane	ClCCl	YMWUJEATGCHHMB-UHFFFAOYSA-N	1.1,2.0	(*21*)(*40*)
1,1-dichloroethane	CC(Cl)Cl	SCYULBFZEHDVBN-UHFFFAOYSA-N	1.5	(*40*)
1,1,1-trichloroethane	CC(Cl)(Cl)Cl	UOCLXMDMGBRAIB-UHFFFAOYSA-N	1.5	(*40*)
1-chlorobutane	CCCCCl	VFWCMGCRMGJXDK-UHFFFAOYSA-N	1.7,2.2	(*21*)(*40*)
chlorobenzene	Clc1ccccc1	MVPPADPHJFYWMZ-UHFFFAOYSA-N	1.8	(*21*)
1,3-dichloropropane	ClCCCCl	YHRUOJUYPBUZOS-UHFFFAOYSA-N	1.9	(*40*)
1,4-dichlorobutane	ClCCCCCl	KJDRSWPQXHESDQ-UHFFFAOYSA-N	2.0	(*40*)
1,5-dichloropentane	ClCCCCCCl	LBKDGROORAKTLC-UHFFFAOYSA-N	2.2	(*40*)
1-chloropentane	CCCCCCl	SQCZQTSHSZLZIQ-UHFFFAOYSA-N	2.2	(*40*)
2-chloropropane	CC(C)Cl	ULYZAYCEDJDHCC-UHFFFAOYSA-N	2.4	(*40*)
1,2-dichloroethane	ClCCCl	WSLDOOZREJYCGB-UHFFFAOYSA-N	2.4	(*40*)
chlorocyclohexane	ClC1CCCCC1	UNFUYWDGSFDHCW-UHFFFAOYSA-N	2.5,2.6	(*40*)(*20*)
2-chloro-2-methylpropane	CC(C)(C)Cl	NBRKLOOSMBRFMH-UHFFFAOYSA-N	2.6,2.4	(*21*)(*40*)
1-chloroadamantane	Cl[C@]12C[C@H]3C[C@H](C [C@H](C3)C1)C2	OZNXTQSXSHODFR-CHIWXEEVSA-N	2.7	(*40*)

3.9 BROMINE

Common Name	Canonical Smiles	InChIKey	β	References
bromobenzene	Brc1ccccc1	QARVLSVVCXYDNA-UHFFFAOYSA-N	1.4	(*21*)
dibromomethane	BrCBr	FJBFPHVGVWTDIP-UHFFFAOYSA-N	1.5	(*40*)
1,2-dibromoethane	BrCCBr	PAAZPARNPHGIKF-UHFFFAOYSA-N	1.7	(*40*)
1,3-dibromopropane	BrCCCBr	VEFLKXRACNJHOV-UHFFFAOYSA-N	1.9	(*40*)
bromocyclopropane	BrC1CC1	LKXYJYDRLBPHRS-UHFFFAOYSA-N	2.0	(*40*)
1,4-dibromobutane	BrCCCCBr	ULTHEAFYOOPTTB-UHFFFAOYSA-N	2.0	(*40*)
1-bromopropane	CCCBr	CYNYIHKIEHGYOZ-UHFFFAOYSA-N	2.2	(*40*)
bromoethane	CCBr	RDHPKYGYEGBMSE-UHFFFAOYSA-N	2.2	(*40*)
1-bromopentane	CCCCCBr	YZWKKMVJZFACSU-UHFFFAOYSA-N	2.3	(*40*)
2-bromo-2-methylpropane	CC(C)(C)Br	RKSOPLXZQNSWAS-UHFFFAOYSA-N	2.3,2.6	(*21*)(*40*)
2-bromopropane	CC(C)Br	NAMYKGVDVNBCFQ-UHFFFAOYSA-N	2.4	(*40*)
bromocyclohexane	BrC1CCCCC1	AQNQQHJNRPDOQV-UHFFFAOYSA-N	2.5	(*40*)
1-bromoadamantane	Br[C@]12C[C@H]3C[C@H](C [C@H](C3)C1)C2	VQHPRVYDKRESCL-CHIWXEEVSA-N	2.7	(*40*)
1-bromobutane	CCCCBr	MPPPKRYCTPRNTB-UHFFFAOYSA-N	2.7,2.3,2.4	(*21*)(*40*)(*20*)

3.10 IODINE

Common Name	Canonical Smiles	InChIKey	β	References
iodobenzene	Ic1ccccc1	SNHMUERNLJLMHN-UHFFFAOYSA-N	1.5	(*21*)
1,2-diiodoethane	ICCI	GBBZLMLLFVFKJM-UHFFFAOYSA-N	1.6	(*40*)
diidomethane	ICI	NZZFYRREKKOMAT-UHFFFAOYSA-N	1.6	(*40*)
1,3-diiodopropane	ICCCI	AAAXMNYUNVCMCJ-UHFFFAOYSA-N	1.9	(*40*)
iodoethane	CCI	HVTICUPFWKNHNG-UHFFFAOYSA-N	2.0	(*40*)
1,4-diiodobutane	ICCCCI	ROUYUBHVBIKMQO-UHFFFAOYSA-N	2.0	(*40*)
iodomethane	CI	INQOMBQAUSQDDS-UHFFFAOYSA-N	2.0	(*40*)(*20*)
1-iodopentane	CCCCCI	BLXSFCHWMBESKV-UHFFFAOYSA-N	2.2	(*40*)
2-iodopropane	CC(C)I	FMKOJHQHASLBPH-UHFFFAOYSA-N	2.2	(*40*)
2-iodo-2-methylpropane	CC(C)(C)I	ANGGPYSFTXVERY-UHFFFAOYSA-N	2.3	(*40*)
iodocyclohexane	IC1CCCCC1	FUCOMWZKWIEKRK-UHFFFAOYSA-N	2.4	(*40*)
1-iodoadamantane	IC12CC3CC(CC(C3)C1)C2	PXVOATXCSSPUEM-CHIWXEEVSA-N	2.6	(*40*)

3.11 SOLID STATE PARAMETERS

Common Name	β	**References**
Diaryl alkyl phosphine oxide	9.6	(*41*)
N-Substituted benzimidazole	9.1	(*41*)
N-Substituted imidazole	8	(*41*)
N,N',N'-Trisubstituted urea	7.9	(*41*)
Primary alkyl amide	7.5	(*41*)
Alkylidene hydrazide	7.4	(*41*)
N-Substituted alkylidene hydrazide	7.3	(*41*)
Alkylidene sulfonamide	7.1	(*41*)
N,N'-Disubstituted hydrazide	7.1	(*41*)
N-Aryl N-alkyl benzamide	6.6	(*41*)
Benzimidazole	6.5	(*41*)
Sulphinamide	6.4	(*41*)
N-Substituted pyrazole	6.2	(*41*)
Thiourea, both Ns secondary	6.2	(*41*)
α,β-Unsaturated aldehyde"	6.2	(*41*)
α,β-Unsaturated carboxylic acid"	6.2	(*41*)
Alkylidene hydrazinecarbodithioate	6.1	(*41*)
N-Aryl secondary amide	6.1	(*41*)
Aryl aldehyde oxime	6.1	(*41*)
N,O-Dialkyl secondary carbamate"	6	(*41*)
α,β-Unsaturated alkyl ester	5.8	(*41*)
Alkyl aryl sulphone	5.7	(*41*)
N-Aryl secondary benzamide	5.5	(*41*)
Primary sulphonamide	5.4	(*41*)
N-Aryl O-alkyl secondary carbamate	5.3	(*41*)
N,O-Dialkyl N-aryl oxime	5	(*41*)
Alkylidene sulphonohydrazide	4.9	(*41*)
Oxime	4.9	(*41*)
Dialkylidene hydrazine	4.8	(*41*)
N,N'-Dialkyl diazo	4.2	(*41*)
N,N'-Diaryl diazo	4	(*41*)
Enol	3.6	(*41*)

Common Name	β	References
N-Alkyl N'-aryl diazo	3.5	(*41*)
Organic azide	3.3	(*41*)
α,β-Unsaturated alkyl ether	3	(*41*)
m-Halophenol	2.9	(*41*)
Alkyl aryl thioether	2.6	(*41*)
Disulphide	2.3	(*41*)
Thiol	1.8 (solution state), 2.3	(*41*)(*42*)
Diaryl thioether	1.5	(*41*)
α,β-Unsaturated secondary amine	0.7	(*41*)

3.12 ANIONS

Common Name	Canonical Smiles	InChIKey	β	References
hexafluorophosphate	F[P-](F)(F)(F)(F)F	LJQLCJWAZJINEB-UHFFFAOYSA-N	7	(*4*)
bistriflylimide anion	C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	NHHWJSXMTZIPES-UHFFFAOYSA-N	7.3	(*4*)
perchlorate	[O-]Cl(=O)(=O)=O	VLTRZXGMWDSKGL-UHFFFAOYSA-M	8.3	(*4*)
iodide	[I-]	XMBWDFGMSWQBCA-UHFFFAOYSA-M	[8.9,9.1]	(*4*)
perherrate	[O-][Re](=O)(=O)=O	WPWXHJFQOFOBAC-UHFFFAOYSA-N	9.4	(*4*)
perfluorobutyl sulfonate	C(C(C(F)(F)S(=O)(=O)[O-])(F)F)(C(F)(F)F)(F)F	JGTNAGYHADQMCM-UHFFFAOYSA-M	9.4	(*4*)
triflate anion	C(F)(F)(F)S(=O)(=O)[O-]	ITMCEJHCFYSIIV-UHFFFAOYSA-M	9.4	(*4*)
hydrogen sulfate	OS(=O)(=O)[O-]	QAOWNCQODCNURD-UHFFFAOYSA-M	10.4	(*4*)
bromide	[Br-]	CPELXLSAUQHCOX-UHFFFAOYSA-M	10.6	(*4*)
nitrate	[N+](=O)([O-])[O-]	NHNBFGGVMKEFGY-UHFFFAOYSA-N	10.7	(*4*)
methanesulfonate	CS(=O)(=O)[O-]	AFVFQIVMOAPDHO-UHFFFAOYSA-M	11.3	(*4*)
chloride	[Cl-]	VEXZGXHMUGYJMC-UHFFFAOYSA-M	12.1	(*4*)
phosphate diester	COP(=O)([O-])OC	KKUKTXOBAWVSHC-UHFFFAOYSA-M	14.3	(*4*)
acetate	CC(=O)[O-]	QTBSBXVTEAMEQO-UHFFFAOYSA-M	15	(*4*)
benzoate	C1=CC=C(C=C1)C(=O)[O-]	WPYMKLBDIGXBTP-UHFFFAOYSA-M	15.1	(*4*)

3.13 ORGANOMETALLIC COMPOUNDS

Common Name	β	**References**
trans-[Ni(F)(2-C_5NF_4)(PEt_3)$_2$]	12	(*43*)
trans-[Ni(F)(2-C_5NF_4)(PCy_3)$_2$]	9.7	(*43*)
trans-[Pd(F)(4-C_5NF_4)(PCy_3)$_2$]	11.6	(*43*)
trans-[Pt(F)2-$C_5NF_2H(CF_3)$(PCy_3)$_2$]	11	(*43*)
Cp_2TiF_2	5.8	(*43*)
Cp_2ZrF_2	4.7	(*43*)
Cp_2HfF_2	4.7	(*43*)
$Cp^*_2TiF_2$	6.9	(*43*)
$Cp^*_2ZrF_2$	5.6	(*43*)
$Cp^*_2HfF_2$	5.1-5.4	(*43*)

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