

Data from Linear and Branched Alkane Thermochemistry

Molecule	HF	B3LYP	ω B97	ω B97X	ω B97X-D	LRC- ω PBEh	M06	M06-2X	M06-HF	PBE	PBE on HF Orbitals	PBEc from PBE	PBEc from PBE on HF Orbitals	HFXPBEC	PBE on HFXPBEC Orbitals
methane	-40.2138679203	-40.5405283560	-40.5208254450	-40.5202599557	-40.5228639602	-40.4884664956	-40.4975295262	-40.5036827349	-40.5082902578	-40.4659242910	-40.4576191428	-0.2999631374	-0.3009002719	-40.5160451920	-40.4559173042
ethane	-79.2601041244	-79.8685382989	-79.8397268568	-79.8364804506	-79.8375171573	-79.7744151579	-79.7902485394	-79.8099672708	-79.8305340238	-79.7354920818	-79.7186809915	-0.5596004866	-0.5610637959	-79.8233257845	-79.7159452235
propane	-118.3078373529	-119.1985379794	-119.1610539651	-119.1548420851	-119.1540955482	-119.0627369545	-119.0869110402	-119.1195993214	-119.1513148112	-119.0075194287	-118.9820204043	-0.8201548524	-0.8221389428	-119.1329792788	-118.9782867281
n-butane	-157.3554375669	-158.5283854870	-158.4832879212	-158.4745614142	-158.4730651779	-158.3510386848	-158.3835644242	-158.4285290042	-158.4724840965	-158.2794322608	-158.2452690523	-1.0808335049	-1.0833189860	-158.4425955556	-158.2405605919
n-pentane	-196.4029809045	-197.8581551007	-197.8043349062	-197.7925209730	-197.7892466075	-197.6391871702	-197.6802434744	-197.7382981751	-197.7927372533	-197.5512311458	-197.5083823367	-1.3415403894	-1.3445258320	-197.7521770753	-197.5027036545
n-hexane	-235.4505035698	-237.1879765435	-237.1266995171	-237.1124737554	-237.1087143672	-236.9274499370	-236.9768973604	-237.0469868530	-237.1143105829	-236.8231314329	-236.7716199773	-1.6022106321	-1.6056925073	-237.0617019174	-236.7649711545
n-heptane	-274.4980687111	-276.5176919276	-276.4475465863	-276.4301302170	-276.4244167908	-276.2155629309	-276.2735108263	-276.3569417402	-276.4341755613	-276.0948532153	-276.0346516145	-1.8629403705	-1.8669271625	-276.3713311143	-276.0270294758
n-octane	-313.5456029152	-315.8474980795	-315.7697932314	-315.7499044389	-315.7435798098	-315.5038194542	-315.5702098921	-315.6651002069	-315.7524542798	-315.3667167398	-315.2978496203	-2.1236262435	-2.1281096357	-315.6808825359	-315.2892587053
isobutane	-157.3559833688	-158.5292662283	-158.4852766662	-158.4763801763	-158.4748792193	-158.3523499572	-158.3843620808	-158.4307477302	-158.4785735913	-158.2806879747	-158.2464247310	-1.0817545543	-1.0842453772	-158.4440341549	-158.2417315767
isopentane	-196.4015848971	-197.8575617288	-197.8061271107	-197.7942894875	-197.7917605073	-197.6392810406	-197.6798854736	-197.7388562253	-197.7987576575	-197.5512778666	-197.5082157672	-1.3432028128	-1.3461504198	-197.7523371178	-197.5026177883
isohexane	-235.4489627655	-237.1872654891	-237.1278393878	-237.1132701513	-237.1097542799	-236.9273836874	-236.9759326615	-237.0480708751	-237.1211507879	-236.8230647881	-236.7712972044	-1.6039268462	-1.6073742496	-237.0617688270	-236.7647325598
isoheptane	-274.4965032790	-276.5169450922	-276.4495780500	-276.4323016578	-276.4277572659	-276.2155395619	-276.2724185603	-276.3572959244	-276.4410641989	-276.0947711033	-276.0343336328	-1.8646254017	-1.8685807370	-276.3713476406	-276.0267916270
isooctane	-313.5365299671	-315.8414108617	-315.7709031444	-315.7497812167	-315.7449864558	-315.5005056604	-315.5721485071	-315.6676879472	-315.7596725968	-315.3631930686	-315.2934102353	-2.1300649978	-2.1343179796	-315.6777630154	-315.2851932097
neopentane	-196.4034820468	-197.8596660956	-197.8103377871	-197.7986964151	-197.7968394383	-197.6420940159	-197.6894860568	-197.7428768105	-197.7854424310	-197.5539268822	-197.5107408507	-1.3446193023	-1.3475453819	-197.7555948891	-197.5051674823
neohexane	-235.4469841187	-237.1860274560	-237.1295908368	-237.1143105725	-237.1108805120	-236.9275137763	-236.9800451285	-237.0508158657	-237.1233291031	-236.8227770583	-236.7707432572	-1.6068305549	-1.6101506598	-237.0624765165	-236.7643377979
neoheptane	-274.4942006995	-276.5154830356	-276.4512529848	-276.4332971737	-276.4290807419	-276.2154224005	-276.2769690876	-276.3596265679	-276.4411001554	-276.0942867892	-276.0335428337	-1.8675405777	-1.8713766977	-276.3717458259	-276.0261621911
3-methylpentane	-235.4468366301	-237.1855918025	-237.1266004091	-237.1118554015	-237.1083313070	-236.9259548617	-236.9775018448	-237.0469600009	-237.1121941542	-236.8216180117	-236.7697446881	-1.6046679445	-1.6080785756	-237.0603111411	-236.7632386065
diisopropyl	-235.4455474585	-237.1848697258	-237.1277425705	-237.1126665927	-237.1092130864	-236.9259691363	-236.9765557579	-237.0483456791	-237.1201806173	-236.8214772766	-236.7694132087	-1.6063604184	-1.6096994563	-237.0606115568	-236.7629833221
hexamethylethane	-313.5286608008	-315.8349229734	-315.7694854039	-315.7470241763	-315.7424586293	-315.4965525962	-315.5704787528	-315.6670632965	-315.7658409505	-315.3582091316	-315.2877539211	-2.1358163577	-2.1396935705	-315.6751745890	-315.2799140696
hydrogen	-0.4998781915	-0.5023726386	-0.5014522191	-0.5015832695	-0.5028599743	-0.5029769649	-0.5000160495	-0.4986250535	-0.4973759656	-0.4999054754	-0.4993495576	-0.0056913488	-0.0059519987	-0.5058580067	-0.4990890139
carbon	-37.6902151826	-37.8602622274	-37.8487666105	-37.8460944102	-37.8424292245	-37.8109495984	-37.8287165069	-37.8431894437	-37.8553206054	-37.7972085749	-37.7933407809	-0.1436972279	-0.1437962591	-37.8345300367	-37.7929136520