

Table S8A. Heck reaction database of ethylene as reactant

Reaction ID	Reaction SMILES
1	<chem>C=C.CCCCC(CC)COc1cc(/C=C/c2ccc(/C=C/c3ccc(/C=C/c4ccc(I)cc4)cc3)cc2)c(OCC(CC)CCCC)cc1</chem> <chem>C>>C=Cc1ccc(/C=C/c2ccc(/C=C/c3ccc(/C=C/c4cc(OCC(CC)CCCC)c(C)cc4OCC(CC)CCCC)cc3)cc2)</chem>
2	<chem>C=C.O=Cc1ccc(Br)cc1>>C=Cc1ccc(C=O)cc1</chem>
3	<chem>C=C.COC(=O)c1cccc(C)c1Br>>C=Cc1c(C)cccc1C(=O)OC</chem>
4	<chem>C=C.COC(=O)c1ccc(NC(C)=O)c(Br)c1>>C=Cc1cc(C(=O)OC)ccc1NC(C)=O</chem>
5	<chem>C=C.COc1ccc(Br)cc1>>C=Cc1ccc(OC)cc1</chem>
6	<chem>C=C.O=C(CC(=O)C(F)(F)F)c1ccc(Br)s1>>C=Cc1ccc(C(=O)CC(=O)C(F)(F)F)s1</chem>
7	<chem>C=C.NC(=O)c1cc(Cl)ccc1Br>>C=Cc1ccc(Cl)cc1C(N)=O</chem>
8	<chem>C=C.O=[N+][O-]c1cc(Cl)ccc1Br>>C=Cc1ccc(Cl)cc1[N+](=O)[O-]</chem>
9	<chem>C=C.CCOc1ccc(Br)cc1>>C=Cc1ccc(OCC)cc1</chem>
10	<chem>C=C.Cc1ccc(C(N)=O)c(Br)c1>>C=Cc1cc(C)ccc1C(N)=O</chem>
11	<chem>C=C.Cn1cc(I)cn1>>C=Cc1cnn(C)c1</chem>
12	<chem>C=C.CC(C)(C)OC(=O)n1c(CCl)cc2ccccc2n1>>C=CCc1cc2ccccc2n1C(=O)OC(C)(C)C</chem>
13	<chem>C=C.COc1cc2c(cc1Br)NC(=O)c1ccc(Cl)cc1N2>>C=Cc1cc2c(cc1OC)Nc1cc(Cl)ccc1C(=O)N2</chem>
14	<chem>C=C.O=C(CC(=O)C(F)(F)F)c1ccc(Br)cc1>>C=Cc1ccc(C(=O)CC(=O)C(F)(F)F)cc1</chem>
15	<chem>C=C.Oc1cccc(I)c1>>C=Cc1cccc(O)c1</chem>
16	<chem>C=C.NC(=O)c1ccc(Cl)cc1Br>>C=Cc1cc(Cl)ccc1C(N)=O</chem>
17	<chem>Br1ccc2ccccc2c1.C=C>>C=Cc1ccc2ccccc2c1</chem>
18	<chem>C=C.COc1ccc(I)cc1OC>>C=Cc1ccc(OC)c(OC)c1</chem>
19	<chem>C=C.COC(=O)c1ccc(C)cc1Br>>C=Cc1cc(C)ccc1C(=O)OC</chem>
20	<chem>C=C.COC(=O)c1ccc2cc(Br)ccc2c1>>C=Cc1ccc2cc(C(=O)OC)ccc2c1</chem>
21	<chem>C=C.CCOC(=O)c1cc(Br)ccc1C>>C=Cc1ccc(C)c(C(=O)OCC)c1</chem>
22	<chem>C=C.CC(=O)c1cccc(Br)c1>>C=Cc1cccc(C(C)=O)c1</chem>
23	<chem>C=C.Clc1ccc(Br)cc1>>C=Cc1ccc(Cl)cc1</chem>
24	<chem>C=C.CC(=O)c1cccc1Br>>C=Cc1cccc1C(C)=O</chem>
25	<chem>C=C.Cc1ccc(Cl)cc1>>C=Cc1ccc(C)cc1</chem>
26	<chem>C=C.FC(F)(F)c1cccc(CCl)c1>>C=CCc1cccc(C(F)(F)F)c1</chem>
27	<chem>C=C.CC(=O)Nc1cc(Cl)ccc1Br>>C=Cc1ccc(Cl)cc1NC(C)=O</chem>
28	<chem>Br1cnc2ncnc12.C=C>>C=Cc1cnc2ncnc12</chem>
29	<chem>C=C.FC(F)(F)c1cc(Br)cc(C(F)(F)F)c1>>C=Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1</chem>
30	<chem>C=C.COc1cccc(I)c1>>C=Cc1cccc(OC)c1</chem>
31	<chem>C=C.COC(=O)c1cc(OC)ccc1Br>>C=Cc1ccc(OC)cc1C(=O)OC</chem>
32	<chem>C=C.Cc1cc(C)c(CCl)c(C)c1>>C=CCc1c(C)cc(C)cc1C</chem>
33	<chem>C=C.Cc1nc(C)c(I)c(Cl)n1>>C=Cc1c(C)nc(C)nc1Cl</chem>
34	<chem>C=C.COc1ccc2cc(Br)ccc2c1[N+](=O)[O-]>>C=Cc1ccc2c([N+](=O)[O-])c(OC)ccc2c1</chem>
35	<chem>C=C.O=[N+][O-]c1ccc(Br)cc1>>C=Cc1ccc([N+](=O)[O-])cc1</chem>
36	<chem>C=C.Cc1cccc([N+](=O)[O-])c1Br>>C=Cc1c(C)cccc1[N+](=O)[O-]</chem>
37	<chem>C=C.Cc1c(Br)c(C(F)(F)F)nn1C>>C=Cc1c(C(F)(F)F)nn(C)c1C</chem>
38	<chem>Br1ccenc1.C=C>>C=Cc1ccenc1</chem>
39	<chem>C=C.Cc1ccc(Br)c([N+](=O)[O-])c1>>C=Cc1ccc(C)cc1[N+](=O)[O-]</chem>
40	<chem>C=C.O=C(CC(=O)c1cccc(Br)c1)c1cccc1>>C=Cc1cccc(C(=O)CC(=O)c2ccccc2)c1</chem>
41	<chem>C=C.Clc1cc(I)cen1>>C=Cc1ccnc(Cl)c1</chem>
42	<chem>C=C.CC(=O)Nc1cccc(C)c1Br>>C=Cc1c(C)cccc1NC(C)=O</chem>
43	<chem>C=C.ClC1cccc(Br)c1>>C=CC1cccc(Br)c1</chem>
44	<chem>C=C.C=CCCCC(=O)CCCC(C)OC(=O)c1c(OC)cc(OC)cc1OS(=O)(=O)C(F)(F)F>>C=CCCCC(=O)CC</chem> <chem>CC(C)OC(=O)c1c(C=C)cc(OC)cc1OC</chem>
45	<chem>C=C.Clc1ccc(I)cc1>>C=Cc1ccc(Cl)cc1</chem>
46	<chem>C=C.COC(=O)c1ccc(CCl)cc1>>C=CCc1ccc(C(=O)OC)cc1</chem>
47	<chem>C=C.ClC1cccc(-c2ccccc2)cc1>>C=CCc1cccc(-c2ccccc2)cc1</chem>
48	<chem>C=C.COC(=O)c1cc(Br)cc(C(=O)OC)n1>>C=Cc1cc(C(=O)OC)nc(C(=O)OC)c1</chem>
49	<chem>C=C.COC(=O)c1ccc(Cl)cc1Br>>C=Cc1cc(Cl)ccc1C(=O)OC</chem>
50	<chem>C=C.OCc1cccc1I>>C=Cc1cccc1CO</chem>

51 C=C.COc1cccc(CCl)c1>>C=CCc1cccc(OC)c1
52 C=C.FC(F)(F)c1ccc(I)cc1>>C=Cc1ccc(C(F)(F)F)cc1
53 C=C.COc1ccc([N+](=O)[O-])c(Br)c1>>C=Cc1cc(OC)ccc1[N+](=O)[O-]
54 C=C.COC(=O)c1ccc(Br)c([N+](=O)[O-])c1>>C=Cc1ccc(C(=O)OC)cc1[N+](=O)[O-]
55 C=C.O=Cc1cc(Br)ccc1O>>C=Cc1ccc(O)c(C=O)c1
56 C=C.O=C(CC(=O)c1ccc(Br)cc1)c1ccccc1>>C=Cc1ccc(C(=O)CC(=O)c2ccccc2)cc1
57 C=C.CC(=O)Oc1cccc(I)c1>>C=Cc1cccc(OC(C)=O)c1
58 C=C.C=CCCCCCCCCOC(=O)c1c(OC)cc(OC)cc1OS(=O)(=O)C(F)(F)F>>C=CCCCCCCCCOC(=O)c1c(C=C)cc(OC)cc1OC
59 C=C.NC(=O)c1cccc1Br>>C=Cc1cccc1C(N)=O
60 C=C.COc1ccc(CCl)cc1>>C=CCc1ccc(OC)cc1
61 C=C.COC(=O)c1ccc(I)cc1>>C=Cc1ccc(C(=O)OC)cc1
62 C=C.COC(=O)Cc1c(C(=O)OC)c2n(c(=O)c1Br)CCC2O>>C=Cc1c(CC(=O)OC)c(C(=O)OC)c2n(c1=O)CCC2O
63 C=C.N#Cc1cccc(Br)c1>>C=Cc1cccc(C#N)c1
64 C=C.Cc1ccc([C@@H](C)CCO)c(Br)c1>>C=Cc1cc(C)ccc1[C@@H](C)CCO
65 C=C.O=[N+](=[O-])c1cc(I)cc([N+](=O)[O-])c1>>C=Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
66 C=C.CC(=O)c1ccc(I)cc1>>C=Cc1ccc(C(C)=O)cc1
67 C=C.CC(=O)Nc1cc(C)ccc1Br>>C=Cc1ccc(C)cc1NC(C)=O
68 C=C.O=Cc1cc(Br)ccc1[N+](=O)[O-]>>C=Cc1ccc([N+](=O)[O-])c(C=O)c1
69 C=C.O=C(c1ccccc1)c1cccc(Br)c1>>C=Cc1cccc(C(=O)c2ccccc2)c1
70 C=C.O=C1Nc2ccc(I)cc2C1=O>>C=Cc1ccc2c(c1)C(=O)C(=O)N2
71 C=C.ClCc1cccc1>>C=CCc1cccc1
72 C=C.COC(=O)c1cc(Cl)ccc1Br>>C=Cc1ccc(Cl)cc1C(=O)OC
73 C=C.COc1cc(Br)cc(OC)c1>>C=Cc1cc(OC)cc(OC)c1
74 C=C.Cc1ccc(Br)cc1>>C=Cc1ccc(C)cc1
75 C=C.Ic1ccc2[nH]ccc2c1>>C=Cc1ccc2[nH]ccc2c1
76 BrC=Cc1cccc1.C=C>>C=CC=Cc1cccc1
77 C=C.CCCCC(CC)COc1cc(/C=C/c2ccc(/C=C/c3ccc(/C=C/c4ccc(/C=C/c5ccc(I)cc5)cc4)cc3)cc2)c(OC(C)CCCC)cc1C>>C=Cc1ccc(/C=C/c2ccc(/C=C/c3ccc(/C=C/c4ccc(/C=C/c5cc(OC(C)CCCC)c(C)c5OCC(C)CCCC)cc4)cc3)cc2)cc1
78 C=C.Oc1cc(Br)c2oc(-c3ccc(O)c(F)c3)nc2c1>>C=Cc1cc(O)cc2nc(-c3ccc(O)c(F)c3)oc12
79 C=C.Ic1cccc1>>C=Cc1cccc1
80 C=C.COc1cc(I)cc(OC)c1>>C=Cc1cc(OC)cc(OC)c1
81 C=C.CCOP(=O)(Cc1ccc(Br)cc1)OCC>>C=Cc1ccc(CP(=O)(OCC)OCC)cc1
82 C=C.Ic1ccc(-c2ccccc2)cc1>>C=Cc1ccc(-c2ccccc2)cc1
83 Br1ccc(-c2nnc(-c3cccc4ccccc34)o2)cc1.C=C>>C=Cc1ccc(-c2nnc(-c3cccc4ccccc34)o2)cc1
84 C=C.OC(c1ccc(Br)cc1)(C(F)(F)F)C(F)(F)F>>C=Cc1ccc(C(O)(C(F)(F)F)C(F)(F)F)cc1
85 Br1cccc2cccc12.C=C>>C=Cc1cccc2cccc12
86 C=C.CCOC(=O)c1c[nH]c(=O)c(I)c1>>C=Cc1cc(C(=O)OCC)c[nH]c1=O
87 C=C.NC(=O)c1[nH]c2ccc(Br)cc2c1S(=O)(=O)N1CCOCC1>>C=Cc1ccc2[nH]c(C(N)=O)c(S(=O)(=O)N3CCOCC3)c2c1
88 C=C.CC(=O)Nc1ccc(Br)cn1>>C=Cc1ccc(NC(C)=O)nc1
89 C=C.N#Cc1ccc(I)cc1>>C=Cc1ccc(C#N)cc1
90 C=C.Fc1ccc(I)cc1>>C=Cc1ccc(F)cc1
91 C=C.Cc1ccc(I)cc1>>C=Cc1ccc(C)cc1
92 C=C.COc1cccc1Br>>C=Cc1cccc1OC
93 C=C.N#Cc1cccc(I)c1>>C=Cc1cccc(C#N)c1
94 C=C.O=S(=O)(Oc1ccc(I)cc1)C(F)(F)F>>C=Cc1ccc(OS(=O)(=O)C(F)(F)F)cc1
95 C=C.ClCc1cc2ccccc2s1>>C=CCc1cc2ccccc2s1
96 C=C.CC(=O)Nc1ccc(I)cc1>>C=Cc1ccc(NC(C)=O)cc1
97 C=C.O=[N+](=[O-])c1cc(Br)cc([N+](=O)[O-])c1>>C=Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
98 C=C.COc1ccc2cc(Br)ccc2c1>>C=Cc1ccc2cc(OC)ccc2c1
99 C=C.O=C(CC(=O)C(F)(F)F)c1ccc(Br)c2ccccc12>>C=Cc1ccc(C(=O)CC(=O)C(F)(F)F)c2ccccc12
100 C=C.Cc1nsc1I>>C=Cc1scnc1C
101 C=C.CC(=O)c1ccc(Br)cc1>>C=Cc1ccc(C(C)=O)cc1
102 C=C.Nc1ccc(Br)cc1>>C=Cc1ccc(N)cc1
103 Br1cncnc1.C=C>>C=Cc1cncnc1
104 C=C.ClCc1csc2ccccc12>>C=CCc1csc2ccccc12

105 C=C.CC(=O)CC(=O)c1ccc(Br)cc1>>C=Cc1ccc(C(=O)CC(C)=O)cc1
106 BrC1=CCCCC1.C=C>>C=CC1=CCCCC1
107 Br1cc2ccc1CCc1ccc(cc1)CC2.C=C>>C=Cc1cc2ccc1CCc1ccc(cc1)CC2
108 C=C.ClC1cccc(Oc2ccccc2)c1>>C=CCc1cccc(Oc2ccccc2)c1
109 C=C.O/N=C/c1cc(Br)ccc1O>>C=Cc1ccc(O)c(/C=N/O)c1
110 C=C.COC(=O)c1cccc(Br)c1NC(C)=O>>C=Cc1cccc(C(=O)OC)c1NC(C)=O
111 C=C.C=CCCCC1(CCC[C@H](C)OC(=O)c2c(OC)cc(OC)cc2OS(=O)(=O)C(F)(F)F)OCCO1>>C=CCC
CC1(CCC[C@H](C)OC(=O)c2c(C=C)cc(OC)cc2OC)OCCO1
112 C=C.Fc1ccccc1I>>C=Cc1ccccc1F
113 C=C.N#Cc1ccccc1Br>>C=Cc1ccccc1C#N
114 C=C.Fc1cc(Br)ccc1-c1ccccc1>>C=Cc1ccc(-c2ccccc2)c(F)c1
115 C=C.Cc1cccc(I)c1>>C=Cc1cccc(C)c1
116 C=C.Ic1cccc2ccccc12>>C=Cc1cccc2ccccc12
117 C=C.Clc1ccccc1I>>C=Cc1ccccc1Cl
118 C=C.CC(=O)Nc1ccc(C)cc1Br>>C=Cc1cc(C)ccc1NC(C)=O
119 C=C.Oc1cccc(Br)c1>>C=Cc1cccc(O)c1
120 C=C.ClC1cc2ccccc2o1>>C=CCc1cc2ccccc2o1
121 C=C.CC(C)Cc1ccc(Br)cc1>>C=Cc1ccc(CC(C)C)cc1
122 C=C.Fc1ccc(I)cn1>>C=Cc1ccc(F)nc1
123 C=C.N#Cc1ccc(Br)cc1>>C=Cc1ccc(C#N)cc1
124 C=C.COC(=O)c1cccc(NC(C)=O)c1Br>>C=Cc1c(NC(C)=O)cccc1C(=O)OC
125 C=C.Cc1cccc(Br)c1>>C=Cc1cccc(C)c1
126 C=C.C=CCCCCCC(C)OC(=O)c1c(OC)cc(OC)cc1OS(=O)(=O)C(F)(F)F>>C=CCCCCCC(C)OC(=O)c
1c(C=C)cc(OC)cc1OC
127 Br1ccc2c(c1)OCCOCCOCCOCCOCCO2.C=C>>C=Cc1ccc2c(c1)OCCOCCOCCOCCOCCO2
128 C=C.ClC1ccccc1I>>C=CCc1ccccc1I
129 C=C.CC(C)(C)OC(=O)n1cc(CCl)c2ccccc21>>C=CCc1cn(C(=O)OC(C)(C)C)c2ccccc12
130 C=C.O=C(O)c1ccc(I)cc1>>C=Cc1ccc(C(=O)O)cc1
131 C=C.Cc1ccc(S(=O)(=O)n2cccc2CCl)cc1>>C=CCc1cccn1S(=O)(=O)c1ccc(C)cc1
132 C=C.O=[N+](=[O-])c1ccc(I)cc1>>C=Cc1ccc([N+](=O)[O-])cc1
133 C=C.COc1ccc(Br)c(C(N)=O)c1>>C=Cc1ccc(OC)cc1C(N)=O
134 C=C.COc1ccc(I)cc1>>C=Cc1ccc(OC)cc1
135 C=C.COC(=O)c1ccc(Br)c(NC(C)=O)c1>>C=Cc1ccc(C(=O)OC)cc1NC(C)=O
136 C=C.COC(=O)C=CBr>>C=CC=CC(=O)OC
137 C=C.CCCCC(CC)COc1cc(/C=C/c2ccc(/C=C/c3ccc(Br)cc3)cc2)c(OCC(CC)CCCC)cc1C>>C=Cc1ccc(/
C=C/c2ccc(/C=C/c3cc(OCC(CC)CCCC)c(C)cc3OCC(CC)CCCC)cc2)cc1
138 Br1ccc2c(c1)CC2.C=C>>C=Cc1ccc2c(c1)CC2
139 C=C.COc1ccc(Br)c(NC(C)=O)c1>>C=Cc1ccc(OC)cc1NC(C)=O
140 C=C.Cc1ccc([N+](=O)[O-])c(Br)c1>>C=Cc1cc(C)ccc1[N+](=O)[O-]
141 C=C.Ic1cccn1>>C=Cc1cccn1
142 C=C.CC(=O)Nc1ccccc1Br>>C=Cc1ccccc1NC(C)=O
143 C=C.O=Cc1ccc(Br)cc1O>>C=Cc1ccc(C(=O)c(O)c1
144 C=C.COC(=O)c1ccc(Br)cc1>>C=Cc1ccc(C(=O)OC)cc1
145 C=C.COC(=O)c1cccc(Br)c1[N+](=O)[O-]>>C=Cc1cccc(C(=O)OC)c1[N+](=O)[O-]
146 C=C.Cc1ccccc1Br>>C=Cc1ccccc1C
147 C=C.Cc1cccc(C(N)=O)c1Br>>C=Cc1c(C)cccc1C(N)=O
148 C=C.O=Cc1cccc(Br)c1>>C=Cc1cccc(C=O)c1
149 C=C.Oc1ccc(I)cc1>>C=Cc1ccc(CO)cc1
150 C=C.COc1ccc(NC(C)=O)c(Br)c1>>C=Cc1cc(OC)ccc1NC(C)=O
151 C=C.N#CCc1ccccc1I>>C=Cc1ccccc1CC#N
152 C=C.Cc1ccccc1I>>C=Cc1ccccc1C
153 Br1cccs1.C=C>>C=Cc1cccs1
154 C=C.Cc1cc(C)c(I)c(C)c1>>C=Cc1c(C)cc(C)cc1C
155 C=C.COC(=O)c1ccccc1Br>>C=Cc1ccccc1C(=O)OC
156 C=C.CC(C)(C)C1CC=C(Br)CC1>>C=CC1=CCC(C(C)(C)C)CC1
157 C=C.Clc1cccc(I)c1>>C=Cc1cccc(Cl)c1