

Benzenepropanoic acid, ethyl ester

Other names:	Hydrocinnamic acid, ethyl ester Ethyl dihydrocinnamate Ethyl hydrocinnamate Ethyl 3-phenylpropanoate Ethyl 3-phenylpropionate Ethyl benzenepropanoate Ethylphenyl propanoate Ethyl 2,3-dihydrocinnamate ethyl 3-phenylpropionate
Inchi:	InChI=1S/C11H14O2/c1-2-13-11(12)9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
InchiKey:	JAGZUIGGHGTFHO-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCOC(=O)CCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	2021-28-5

Physical Properties

Property code	Value	Unit	Source
chl	-5906.30 ± 4.70	kJ/mol	NIST Webbook
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1320.00		NIST Webbook

rinpol	1357.00	NIST Webbook
rinpol	1351.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1349.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1350.00	NIST Webbook
rinpol	1370.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1350.00	NIST Webbook
rinpol	1355.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1390.40	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1347.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1320.00	NIST Webbook
rinpol	1350.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1360.00	NIST Webbook
rinpol	1353.00	NIST Webbook
rinpol	1320.00	NIST Webbook
ripol	1846.00	NIST Webbook
ripol	1914.00	NIST Webbook
ripol	1854.00	NIST Webbook
ripol	1909.00	NIST Webbook
ripol	1879.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1861.00	NIST Webbook
ripol	1903.00	NIST Webbook
ripol	1905.00	NIST Webbook
ripol	1908.00	NIST Webbook
ripol	1862.00	NIST Webbook
ripol	1908.00	NIST Webbook
ripol	1886.00	NIST Webbook
ripol	1886.00	NIST Webbook
ripol	1904.00	NIST Webbook
ripol	1892.00	NIST Webbook
ripol	1872.00	NIST Webbook
ripol	1878.00	NIST Webbook
ripol	1899.00	NIST Webbook
ripol	1892.00	NIST Webbook
ripol	1897.00	NIST Webbook

ripol	1897.00		NIST Webbook
ripol	1903.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	520.40 ± 1.00	K	NIST Webbook
tb	520.40	K	NIST Webbook
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.37	J/molxK	763.32	Joback Method
cpg	410.76	J/molxK	728.44	Joback Method
cpg	399.42	J/molxK	693.56	Joback Method
cpg	387.33	J/molxK	658.68	Joback Method
cpg	374.48	J/molxK	623.81	Joback Method
cpg	360.84	J/molxK	588.93	Joback Method
cpg	346.39	J/molxK	554.05	Joback Method
cpl	286.60	J/molxK	298.00	NIST Webbook
dvisc	0.0002569	Paxs	513.76	Joback Method
dvisc	0.0003432	Paxs	473.47	Joback Method
dvisc	0.0004838	Paxs	433.18	Joback Method
dvisc	0.0007317	Paxs	392.89	Joback Method
dvisc	0.0012165	Paxs	352.60	Joback Method
dvisc	0.0023060	Paxs	312.31	Joback Method
dvisc	0.0002006	Paxs	554.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2021285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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