Benzenepropanoic acid, methyl ester

Other names:	Hydrocinnamic acid, methyl ester
	«beta»-Phenylpropionic acid methyl ester
	Methyl «beta»-phenylpropionate
	Methyl hydrocinnamate
	Methyl 3-phenylpropanoate
	Methyl 3-phenylpropionate
	Methyl benzenepropanoate
	Methyl dihydrocinnamate
	Methyl ester of «beta»-Phenylpropionic acid
	Methyl phenylpropionate
	3-Phenylpropanoic acid methyl ester
	Dihydromethyl cinnamate
	methyl (3-phenyl) propanoate
Inchi:	InChI=1S/C10H12O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3
InchiKey:	RPUSRLKKXPQSGP-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	COC(=O)CCc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	103-25-3

Physical Properties

Property code	Value	Unit	Source
gf	-88.19	kJ/mol	Joback Method
hf	-258.00	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	1.792		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1258.00		NIST Webbook

rinpol	1246.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	217.51		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1279.10		NIST Webbook
rinpol	1295.20		NIST Webbook
rinpol	1280.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1854.00		NIST Webbook
tb	511.70	K	NIST Webbook
tc	743.85	K	Joback Method
tf	301.04	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.47	J/mol×K	531.17	Joback Method
cpg	314.07	J/mol×K	566.62	Joback Method
cpg	326.90	J/mol×K	602.06	Joback Method
cpg	338.99	J/mol×K	637.51	Joback Method
cpg	350.35	J/mol×K	672.95	Joback Method
cpg	361.01	J/mol×K	708.40	Joback Method
cpg	370.98	J/mol×K	743.85	Joback Method
dvisc	0.0023380	Pa×s	301.04	Joback Method
dvisc	0.0012567	Pa×s	339.39	Joback Method
dvisc	0.0007662	Pa×s	377.75	Joback Method
dvisc	0.0005118	Pa×s	416.11	Joback Method
dvisc	0.0003660	Pa×s	454.46	Joback Method
dvisc	0.0002757	Pa×s	492.81	Joback Method
dvisc	0.0002164	Pa×s	531.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103253&Units=SI

Legend

cpg:	Ideal gas 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
ie:	Ionization energy
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