Benzenepropanoic acid, «alpha»-hydroxy-, methyl ester

Other names: Lactic acid, 3-phenyl-, methyl ester
«beta»-Phenyllactic acid methyl ester
Methyl 2-hydroxy-3-phenylpropionate
Methyl 2-hydroxy-3-phenylpropanoate

Inchi: InChI=1S/C10H12O3/c1-13-10(12)9(11)7-8-5-3-2-4-6-8/h2-6,9,11H,7H2,1H3

InchiKey: NMPPJJIBQQCOOI-UHFFFAOYSA-N

Formula: C10H12O3

SMILES: COC(=O)C(O)Cc1ccccc1

Mol. weight [g/mol]: 180.20

CAS: 13674-16-3

Physical Properties

Property code	Value	Unit	Source
gf	-227.45	kJ/mol	Joback Method
hf	-415.51	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.763		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1634.20		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	622.91	K	Joback Method
tc	825.20	K	Joback Method
tf	346.86	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	351.77	J/mol×K	622.91	Joback Method
cpg	363.16	J/mol×K	656.63	Joback Method
cpg	373.87	J/mol×K	690.34	Joback Method
cpg	383.91	J/mol×K	724.06	Joback Method
cpg	393.31	J/mol×K	757.77	Joback Method
cpg	402.07	J/mol×K	791.49	Joback Method
cpg	410.23	J/mol×K	825.20	Joback Method
dvisc	0.0050139	Pa×s	346.86	Joback Method
dvisc	0.0015849	Pa×s	392.87	Joback Method
dvisc	0.0006378	Pa×s	438.88	Joback Method
dvisc	0.0003051	Pa×s	484.88	Joback Method
dvisc	0.0001658	Pa×s	530.89	Joback Method
dvisc	0.0000993	Pa×s	576.90	Joback Method
dvisc	0.0000642	Pa×s	622.91	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13674163&Units=SI
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

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume