Isobutyl 3-hydroxy-2-methylenebutanoate

Other names: Butanoic acid, 3-hydroxy-2-methylene-, 2-methylpropyl ester
Inchi: InChI=1S/C9H16O3/c1-6(2)5-12-9(11)7(3)8(4)10/h6,8,10H,3,5H2,1-2,4H3
InchiKey: YWLLUDSCDSOEDO-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: C=C(C(=O)OCC(C)C)C(C)O
Mol. weight [g/mol]: 172.22
CAS: 80758-68-5

Physical Properties

Property code	Value	Unit	Source
gf	-271.43	kJ/mol	Joback Method
hf	-521.04	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	60.10	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.123		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1181.80		NIST Webbook
rinpol	1177.00		NIST Webbook
tb	569.47	K	Joback Method
tc	748.49	K	Joback Method
tf	278.45	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.60	J/mol×K	569.47	Joback Method
cpg	372.22	J/mol×K	599.31	Joback Method
cpg	383.33	J/mol×K	629.14	Joback Method
cpg	393.93	J/mol×K	658.98	Joback Method
cpg	404.03	J/mol×K	688.82	Joback Method
cpg	413.65	J/mol×K	718.65	Joback Method

cpg	422.79	J/mol×K	748.49	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=C80758685&Units=SI

Legend

cpg:	Ideal gas heat capacity
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