Isopentyl 3-hydroxy-2-methylenebutanoate

Other names: 2-Methylbutyl 3-hydroxy-2-methylenebutanoate
Inchi: InChI=1S/C10H18O3/c1-7(2)5-6-13-10(12)8(3)9(4)11/h7,9,11H,3,5-6H2,1-2,4H3
InchiKey: URBTVTZTLQVLCO-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: C=C(C(=O)OCCC(C)C)C(C)O
Mol. weight [g/mol]: 186.25
CAS: 80758-69-6

Physical Properties

Property code	Value	Unit	Source
gf	-263.01	kJ/mol	Joback Method
hf	-541.68	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.513		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1284.20		NIST Webbook
rinpol	1284.20		NIST Webbook
tb	592.35	K	Joback Method
tc	769.87	K	Joback Method
tf	289.72	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.31	J/mol×K	592.35	Joback Method
cpg	420.69	J/mol×K	621.94	Joback Method
cpg	432.51	J/mol×K	651.52	Joback Method
cpg	443.79	J/mol×K	681.11	Joback Method
cpg	454.54	J/mol×K	710.70	Joback Method
cpg	464.76	J/mol×K	740.29	Joback Method

cpg	474.46	J/mol×K	769.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80758696&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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