2-methylallyl isobutyrate

Other names: 2-Methylpropanoic acid, 2-methyl-, 2-propenyl ester
Inchi: InChI=1S/C8H14O2/c1-6(2)5-10-8(9)7(3)4/h7H,1,5H2,2-4H3
InchiKey: SMCDNXLLJDMHQF-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: C=C(C)COC(=O)C(C)C
Mol. weight [g/mol]: 142.20
CAS: 816-73-9

Physical Properties

Property code	Value	Unit	Source
gf	-140.59	kJ/mol	Joback Method
hf	-342.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	41.58	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.762		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	927.40		NIST Webbook
rinpol	927.40		NIST Webbook
tb	454.85	K	Joback Method
tc	640.80	K	Joback Method
tf	221.36	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.11	J/mol×K	454.85	Joback Method
cpg	275.28	J/mol×K	485.84	Joback Method
cpg	286.96	J/mol×K	516.83	Joback Method
cpg	298.16	J/mol×K	547.83	Joback Method
cpg	308.88	J/mol×K	578.82	Joback Method
cpg	319.14	J/mol×K	609.81	Joback Method

cpg	328.94	J/mol×K	640.80	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=C816739&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