2-Butenoic acid, 3-methyl-, 2-methylpropyl ester

Other names: 3-Methyl-2-butenoic acid, 2-methylpropyl ester
isobutyl 3-methyl-2-butenoate
Isobutyl 3-methylbut-2-enoate
Inchi: InChI=1S/C9H16O2/c1-7(2)5-9(10)11-6-8(3)4/h5,8H,6H2,1-4H3
InchiKey: OORIYKITSHAVJG-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC(C)=CC(=O)OCC(C)C
Mol. weight [g/mol]: 156.22
CAS: 30434-54-9

Physical Properties

Property code	Value	Unit	Source
gf	-139.79	kJ/mol	Joback Method
hf	-371.74	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	54.70 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
tb	485.21	K	Joback Method
tc	674.06	K	Joback Method
tf	229.31	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.09	J/mol×K	485.21	Joback Method
cpg	319.56	J/mol×K	516.68	Joback Method
cpg	332.44	J/mol×K	548.16	Joback Method
cpg	344.74	J/mol×K	579.63	Joback Method

cpg	356.48	J/mol×K	611.11	Joback Method
cpg	367.66	J/mol×K	642.58	Joback Method
cpg	378.31	J/mol×K	674.06	Joback Method

Sources

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=C30434549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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