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

Other names: Isobutyl 2-methyl-2-butenoate
Isobutyl tiglate
Inchi: InChI=1S/C9H16O2/c1-5-8(4)9(10)11-6-7(2)3/h5,7H,6H2,1-4H3/b8-5+
InchiKey: XDEGQMQKHFPBEW-VMPITWQZSA-N
Formula: C9H16O2
SMILES: CC=C(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 156.22
CAS: 66917-61-1

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	44.43	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1357.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66917611&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume