2-Butenoic acid, 2-methylpropyl ester

Other names: Isobutyl 2-butenoate
2-methylpropyl crotonate
Inchi: InChI=1S/C8H14O2/c1-4-5-8(9)10-6-7(2)3/h4-5,7H,6H2,1-3H3/b5-4+
InchiKey: XDOWKOALJBOBBL-SNAWJCMRSA-N
Formula: C8H14O2
SMILES: CC=CC(=O)OCC(C)C
Mol. weight [g/mol]: 142.20
CAS: 589-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-139.66	kJ/mol	Joback Method
hf	-341.31	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	42.13	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.762		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	975.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
tb	462.45	K	Joback Method
tc	649.84	K	Joback Method
tf	232.00	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.44	J/mol×K	462.45	Joback Method
cpg	275.69	J/mol×K	493.68	Joback Method
cpg	287.40	J/mol×K	524.91	Joback Method

cpg	298.61	J/mol×K	556.15	Joback Method
cpg	309.31	J/mol×K	587.38	Joback Method
cpg	319.53	J/mol×K	618.61	Joback Method
cpg	329.27	J/mol×K	649.84	Joback Method
dvisc	0.0045131	Pa×s	232.00	Joback Method
dvisc	0.0018620	Pa×s	270.41	Joback Method
dvisc	0.0009575	Pa×s	308.82	Joback Method
dvisc	0.0005704	Pa×s	347.23	Joback Method
dvisc	0.0003767	Pa×s	385.63	Joback Method
dvisc	0.0002682	Pa×s	424.04	Joback Method
dvisc	0.0002021	Pa×s	462.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589662&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
dvisc:	Dynamic viscosity
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

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