

3-methylbutyl crotonate

Other names:	2-Butenoic acid, 3-methyl, butyl ester Isopentyl 2-butenate (E)-2-Butenoic acid 3-methylbutyl ester
Inchi:	InChI=1S/C9H16O2/c1-4-5-9(10)11-7-6-8(2)3/h4-5,8H,6-7H2,1-3H3/b5-4+
InchiKey:	JAVOYFHBJFLMRQ-SNAWJCMRSA-N
Formula:	C9H16O2
SMILES:	CC=CC(=O)OCCC(C)C
Mol. weight [g/mol]:	156.22
CAS:	25415-77-4

Physical Properties

Property code	Value	Unit	Source
chl	-5327.50 ± 2.90	kJ/mol	NIST Webbook
gf	-131.24	kJ/mol	Joback Method
hf	-447.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-501.00 ± 3.00	kJ/mol	NIST Webbook
hfus	18.53	kJ/mol	Joback Method
hvap	54.00	kJ/mol	NIST Webbook
hvap	54.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	485.33	K	Joback Method
tc	670.77	K	Joback Method
tf	243.27	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.21	J/mol×K	485.33	Joback Method
cpg	319.47	J/mol×K	516.24	Joback Method
cpg	332.17	J/mol×K	547.14	Joback Method
cpg	344.30	J/mol×K	578.05	Joback Method
cpg	355.88	J/mol×K	608.96	Joback Method
cpg	366.93	J/mol×K	639.87	Joback Method
cpg	377.46	J/mol×K	670.77	Joback Method
dvisc	0.0044834	Pa×s	243.27	Joback Method
dvisc	0.0018217	Pa×s	283.61	Joback Method
dvisc	0.0009263	Pa×s	323.96	Joback Method
dvisc	0.0005471	Pa×s	364.30	Joback Method
dvisc	0.0003589	Pa×s	404.64	Joback Method
dvisc	0.0002542	Pa×s	444.99	Joback Method
dvisc	0.0001906	Pa×s	485.33	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=C25415774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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