

2-Butenoic acid, 2-methyl-, 3-methylbutyl ester, (E)-

Other names:	3-Methylbutyl angelate Isoamyl angelate Isopentyl (E)-2-methylbut-2-enoate isopentyl 2-methylcrotonate
Inchi:	InChI=1S/C10H18O2/c1-5-9(4)10(11)12-7-6-8(2)3/h5,8H,6-7H2,1-4H3/b9-5+
InchiKey:	ZARFDQHJMNVNLE-WEVVVXLNSA-N
Formula:	C10H18O2
SMILES:	<chem>CC=C(C)C(=O)OCCC(C)C</chem>
Mol. weight [g/mol]:	170.25
CAS:	41519-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-131.37	kJ/mol	Joback Method
hf	-392.38	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1195.80		NIST Webbook
rinpol	1168.00		NIST Webbook
tb	508.09	K	Joback Method
tc	694.82	K	Joback Method
tf	240.58	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.82	J/mol×K	508.09	Joback Method
cpg	365.21	J/mol×K	539.21	Joback Method
cpg	378.95	J/mol×K	570.33	Joback Method
cpg	392.08	J/mol×K	601.46	Joback Method
cpg	404.60	J/mol×K	632.58	Joback Method
cpg	416.53	J/mol×K	663.70	Joback Method
cpg	427.88	J/mol×K	694.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41519180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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