Butanoic acid, 3-methyl-, 3-methyl-3-butenyl ester

Other names:	3-Methyl-3-buten-1-yl 3-methylbutanoate
	3-Methyl-3-butenyl isovalerate
	3-Methyl-but-3-enyl isovalerate
	3-Methylbutanoic acid, 3-methyl-3-butenyl ester
	3-Methyl butanoate, 3-methyl-3-butenyl
	3-Methyl-3-butenyl 3-methyl butanoate
	3-methylbut-3-en-1-yl 3-methylbutanoate
Inchi:	InChI=1S/C10H18O2/c1-8(2)5-6-12-10(11)7-9(3)4/h9H,1,5-7H2,2-4H3
InchiKey:	TYOOXFQTUDXXCL-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=C(C)CCOC(=O)CC(C)C
Mol. weight [g/mol]:	170.25
CAS:	54410-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-123.75	kJ/mol	Joback Method
hf	-384.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1115.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1372.00		NIST Webbook

tb	500.61	K	Joback Method
tc	682.86	K	Joback Method
tf	243.90	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.92	J/mol×K	500.61	Joback Method
cpg	364.09	J/mol×K	530.98	Joback Method
cpg	377.66	J/mol×K	561.36	Joback Method
cpg	390.66	J/mol×K	591.73	Joback Method
cpg	403.09	J/mol×K	622.11	Joback Method
cpg	414.96	J/mol×K	652.48	Joback Method
cpg	426.29	J/mol×K	682.86	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=C54410945&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume