3-methyl-3-butenyl butanoate

Other names: 3-methyl-but-3-en-1-yl butanoate
Inchi: InChI=1S/C9H16O2/c1-4-5-9(10)11-7-6-8(2)3/h2,4-7H2,1,3H3
InchiKey: QXWHISNFDZLFAV-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: C=C(C)CCOC(=O)CCC
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-129.73	kJ/mol	Joback Method
hf	-358.25	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1063.00		NIST Webbook
ripol	1330.00		NIST Webbook
tb	478.17	K	Joback Method
tc	658.40	K	Joback Method
tf	247.63	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.33	J/mol×K	478.17	Joback Method
cpg	318.20	J/mol×K	508.21	Joback Method
cpg	330.57	J/mol×K	538.25	Joback Method
cpg	342.43	J/mol×K	568.28	Joback Method
cpg	353.79	J/mol×K	598.32	Joback Method

cpg	364.67	J/mol×K	628.36	Joback Method
cpg	375.07	J/mol×K	658.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R238078&Units=SI

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