2-Butenoic acid, 3-methyl-, butyl ester

Other names:	3-Methyl-2-butenoic acid, butyl ester
	Butyl 3-methylbut-2-enoate
	butyl 3-methyl-2-butenoate
Inchi:	InChI=1S/C9H16O2/c1-4-5-6-11-9(10)7-8(2)3/h7H,4-6H2,1-3H3
InchiKey:	IJZWZSGPEJOCHI-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCCCOC(=O)C=C(C)C
Mol. weight [g/mol]:	156.22
CAS:	54056-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-137.35	kJ/mol	Joback Method
hf	-366.46	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	56.60 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
tb	485.65	K	Joback Method
tc	670.48	K	Joback Method
tf	244.31	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.90	J/mol×K	485.65	Joback Method
cpg	319.01	J/mol×K	516.46	Joback Method
cpg	331.57	J/mol×K	547.26	Joback Method
cpg	343.57	J/mol×K	578.07	Joback Method

cpg	355.04	J/mol×K	608.87	Joback Method
cpg	365.99	J/mol×K	639.68	Joback Method
cpg	376.43	J/mol×K	670.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54056518&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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