3-Methyl-2-butenoic acid, 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]: 156.23

Physical Properties

Property code	Value	Unit	Source
af	0.5204		Cheméo Relay (1.0)
hf	-451.88	kJ/mol	Cheméo Relay (1.0)
hfus	20.74	kJ/mol	Joback Method
hvap	56.60 ± 0.30	kJ/mol	NIST Webbook
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-2.79		Cheméo Relay (1.0)
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	459.02	K	Cheméo Relay (1.0)
tc	645.82	K	Cheméo Relay (1.0)
tf	220.01	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54056518&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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