

Butanoic acid, 1-methyl-3-butenyl ester

Inchi:	InChI=1S/C9H16O2/c1-4-6-8(3)11-9(10)7-5-2/h4,8H,1,5-7H2,2-3H3
InchiKey:	GBDHZZRHBRV VII-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CCC(C)OC(=O)CCC
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-123.62	kJ/mol	Joback Method
hf	-353.74	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	43.73	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.294		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1006.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	1007.00		NIST Webbook
tb	477.85	K	Joback Method
tc	658.67	K	Joback Method
tf	246.59	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.61	J/molxK	477.85	Joback Method
cpg	318.63	J/molxK	507.99	Joback Method
cpg	331.13	J/molxK	538.12	Joback Method
cpg	343.12	J/molxK	568.26	Joback Method
cpg	354.60	J/molxK	598.39	Joback Method
cpg	365.59	J/molxK	628.53	Joback Method

cpg	376.08	J/mol×K	658.67	Joback Method
dvisc	0.0043503	Paxs	246.59	Joback Method
dvisc	0.0019129	Paxs	285.13	Joback Method
dvisc	0.0010229	Paxs	323.68	Joback Method
dvisc	0.0006250	Paxs	362.22	Joback Method
dvisc	0.0004198	Paxs	400.76	Joback Method
dvisc	0.0003024	Paxs	439.31	Joback Method
dvisc	0.0002296	Paxs	477.85	Joback Method

Sources

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=R28536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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