

Butanoic acid, 3-butenyl ester

Inchi:	InChI=1S/C8H14O2/c1-3-5-7-10-8(9)6-4-2/h3H,1,4-7H2,2H3
InchiKey:	VDMZXZOJKWISSE-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=CCCOC(=O)CCC
Mol. weight [g/mol]:	142.20
CAS:	21698-32-8

Physical Properties

Property code	Value	Unit	Source
gf	-129.60	kJ/mol	Joback Method
hf	-327.82	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	961.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	972.00		NIST Webbook
tb	455.41	K	Joback Method
tc	633.98	K	Joback Method
tf	250.32	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.07	J/molxK	455.41	Joback Method
cpg	316.89	J/molxK	604.22	Joback Method
cpg	306.99	J/molxK	574.46	Joback Method
cpg	296.66	J/molxK	544.69	Joback Method
cpg	285.90	J/molxK	514.93	Joback Method

cpg	274.71	J/mol×K	485.17	Joback Method
cpg	326.37	J/mol×K	633.98	Joback Method
dvisc	0.0002547	Paxs	455.41	Joback Method
dvisc	0.0003249	Paxs	421.23	Joback Method
dvisc	0.0004328	Paxs	387.05	Joback Method
dvisc	0.0006093	Paxs	352.87	Joback Method
dvisc	0.0009231	Paxs	318.68	Joback Method
dvisc	0.0015454	Paxs	284.50	Joback Method
dvisc	0.0029783	Paxs	250.32	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=C21698328&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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