

Propanoic acid, 1-methyl-3-butenyl ester

Inchi:	InChI=1S/C8H14O2/c1-4-6-7(3)10-8(9)5-2/h4,7H,1,5-6H2,2-3H3
InchiKey:	QTJLXWLLLXXECC-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=CCC(C)OC(=O)CC
Mol. weight [g/mol]:	142.20

Physical Properties

Property code	Value	Unit	Source
gf	-132.04	kJ/mol	Joback Method
hf	-333.10	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.904		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	926.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	913.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1197.00		NIST Webbook
tb	454.97	K	Joback Method
tc	637.48	K	Joback Method
tf	235.32	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.19	J/molxK	454.97	Joback Method

cpg	318.44	J/molxK	607.06	Joback Method
cpg	308.30	J/molxK	576.64	Joback Method
cpg	297.72	J/molxK	546.22	Joback Method
cpg	286.67	J/molxK	515.81	Joback Method
cpg	275.17	J/molxK	485.39	Joback Method
cpg	328.12	J/molxK	637.48	Joback Method
dvisc	0.0002428	Paxs	454.97	Joback Method
dvisc	0.0003181	Paxs	418.36	Joback Method
dvisc	0.0004389	Paxs	381.75	Joback Method
dvisc	0.0006484	Paxs	345.14	Joback Method
dvisc	0.0010509	Paxs	308.54	Joback Method
dvisc	0.0019397	Paxs	271.93	Joback Method
dvisc	0.0043324	Paxs	235.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R113741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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