

Butanoic acid, 2-chloro, 2-propenyl ester

Inchi:	InChI=1S/C7H11ClO2/c1-3-5-10-7(9)6(8)4-2/h3,6H,1,4-5H2,2H3
InchiKey:	TZIYTVFUJREYDE-UHFFFAOYSA-N
Formula:	C7H11ClO2
SMILES:	C=CCOC(=O)C(Cl)CC
Mol. weight [g/mol]:	162.61

Physical Properties

Property code	Value	Unit	Source
gf	-152.39	kJ/mol	Joback Method
hf	-328.20	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	43.66	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.733		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	994.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1028.00		NIST Webbook
ripol	1546.00		NIST Webbook
ripol	1514.00		NIST Webbook
tb	469.52	K	Joback Method
tc	660.02	K	Joback Method
tf	253.97	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.56	J/mol×K	469.52	Joback Method
cpg	258.99	J/mol×K	501.27	Joback Method
cpg	268.98	J/mol×K	533.02	Joback Method
cpg	278.52	J/mol×K	564.77	Joback Method

cpg	287.63	J/mol×K	596.52	Joback Method
cpg	296.31	J/mol×K	628.27	Joback Method
cpg	304.57	J/mol×K	660.02	Joback Method
dvisc	0.0039384	Paxs	253.97	Joback Method
dvisc	0.0019112	Paxs	289.89	Joback Method
dvisc	0.0010878	Paxs	325.82	Joback Method
dvisc	0.0006924	Paxs	361.75	Joback Method
dvisc	0.0004783	Paxs	397.67	Joback Method
dvisc	0.0003512	Paxs	433.60	Joback Method
dvisc	0.0002704	Paxs	469.52	Joback Method

Sources

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=R28625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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