

3-Chloropropionic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C6H8Cl2O2/c7-3-1-5-10-6(9)2-4-8/h1,3H,2,4-5H2/b3-1+
InchiKey:	CSADUUPDAFPXAX-HNQUOIGGSA-N
Formula:	C6H8Cl2O2
SMILES:	O=C(CCCl)OCC=CCl
Mol. weight [g/mol]:	183.03

Physical Properties

Property code	Value	Unit	Source
gf	-177.92	kJ/mol	Joback Method
hf	-326.23	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.911		Crippen Method
mcvol	123.020	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1172.00		NIST Webbook
tb	491.99	K	Joback Method
tc	691.29	K	Joback Method
tf	284.30	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.20	J/molxK	491.99	Joback Method
cpg	239.89	J/molxK	525.21	Joback Method
cpg	248.13	J/molxK	558.42	Joback Method
cpg	255.95	J/molxK	591.64	Joback Method
cpg	263.35	J/molxK	624.86	Joback Method
cpg	270.36	J/molxK	658.07	Joback Method
cpg	276.97	J/molxK	691.29	Joback Method
dvisc	0.0026290	Paxs	284.30	Joback Method
dvisc	0.0014478	Paxs	318.92	Joback Method

dvisc	0.0008961	Paxs	353.53	Joback Method
dvisc	0.0006042	Paxs	388.15	Joback Method
dvisc	0.0004345	Paxs	422.76	Joback Method
dvisc	0.0003285	Paxs	457.38	Joback Method
dvisc	0.0002583	Paxs	491.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299221&Units=SI

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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