

Cyclopropanecarboxylic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C7H9ClO2/c8-4-1-5-10-7(9)6-2-3-6/h1,4,6H,2-3,5H2/b4-1+
InchiKey:	QAJSCZWJFSRULT-DAFODLJHSA-N
Formula:	C7H9ClO2
SMILES:	O=C(OCC=CC)C1CC1
Mol. weight [g/mol]:	160.60

Physical Properties

Property code	Value	Unit	Source
gf	-96.82	kJ/mol	Joback Method
hf	-258.33	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	44.59	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.692		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	855.00		NIST Webbook
rinpol	855.00		NIST Webbook
tb	484.18	K	Joback Method
tc	690.70	K	Joback Method
tf	283.59	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.83	J/molxK	484.18	Joback Method
cpg	244.04	J/molxK	518.60	Joback Method
cpg	254.55	J/molxK	553.02	Joback Method
cpg	264.40	J/molxK	587.44	Joback Method
cpg	273.62	J/molxK	621.86	Joback Method
cpg	282.26	J/molxK	656.28	Joback Method
cpg	290.36	J/molxK	690.70	Joback Method
dvisc	0.0018693	Paxs	283.59	Joback Method

dvisc	0.0013034	Paxs	317.02	Joback Method
dvisc	0.0009736	Paxs	350.45	Joback Method
dvisc	0.0007652	Paxs	383.88	Joback Method
dvisc	0.0006250	Paxs	417.32	Joback Method
dvisc	0.0005261	Paxs	450.75	Joback Method
dvisc	0.0004535	Paxs	484.18	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=U299383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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