

Acetoxyacetic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C7H9ClO4/c1-6(9)12-5-7(10)11-4-2-3-8/h2-3H,4-5H2,1H3/b3-2+
InchiKey:	MATWRJSMXKVOPA-NSCUHMNNSA-N
Formula:	C7H9ClO4
SMILES:	CC(=O)OCC(=O)OCC=CCl
Mol. weight [g/mol]:	192.60

Physical Properties

Property code	Value	Unit	Source
gf	-391.49	kJ/mol	Joback Method
hf	-575.93	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	53.83	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.845		Crippen Method
mcvol	132.310	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpola	1245.00		NIST Webbook
tb	553.73	K	Joback Method
tc	752.60	K	Joback Method
tf	337.81	K	Joback Method
vc	0.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.40	J/mol×K	553.73	Joback Method
cpg	326.04	J/mol×K	719.46	Joback Method
cpg	318.39	J/mol×K	686.31	Joback Method
cpg	310.31	J/mol×K	653.17	Joback Method
cpg	301.78	J/mol×K	620.02	Joback Method
cpg	292.81	J/mol×K	586.88	Joback Method
cpg	333.25	J/mol×K	752.60	Joback Method
dvisc	0.0002074	Paxs	553.73	Joback Method
dvisc	0.0002618	Paxs	517.74	Joback Method

dvisc	0.0003420	Paxs	481.76	Joback Method
dvisc	0.0004666	Paxs	445.77	Joback Method
dvisc	0.0006723	Paxs	409.78	Joback Method
dvisc	0.0010392	Paxs	373.80	Joback Method
dvisc	0.0017625	Paxs	337.81	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=U299211&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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