

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

Inchi:	InChI=1S/C10H8Cl2O2/c11-6-3-7-14-10(13)8-4-1-2-5-9(8)12/h1-6H,7H2/b6-3+
InchiKey:	GIMRXOTXLJWYLM-ZZXKWWIFSA-N
Formula:	C10H8Cl2O2
SMILES:	O=C(OCC=CCl)c1cccc1Cl
Mol. weight [g/mol]:	231.07

Physical Properties

Property code	Value	Unit	Source
gf	-41.46	kJ/mol	Joback Method
hf	-183.73	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.249		Crippen Method
mcvol	155.620	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1617.00		NIST Webbook
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tb	615.17	K	Joback Method
tc	846.82	K	Joback Method
tf	368.32	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.06	J/molxK	615.17	Joback Method
cpg	376.11	J/molxK	808.21	Joback Method
cpg	368.12	J/molxK	769.60	Joback Method
cpg	359.46	J/molxK	731.00	Joback Method
cpg	350.08	J/molxK	692.39	Joback Method
cpg	339.96	J/molxK	653.78	Joback Method
cpg	383.47	J/molxK	846.82	Joback Method
dvisc	0.0001722	Paxs	615.17	Joback Method

dvisc	0.0002154	Paxs	574.03	Joback Method
dvisc	0.0002789	Paxs	532.89	Joback Method
dvisc	0.0003771	Paxs	491.75	Joback Method
dvisc	0.0005387	Paxs	450.60	Joback Method
dvisc	0.0008269	Paxs	409.46	Joback Method
dvisc	0.0013966	Paxs	368.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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