

2-Chloromethyl-1,3-dichloro-2-methylpropane

Other names:	2-Chloromethyl-2-methyl-1,3-dichloropropane
Inchi:	InChI=1S/C5H9Cl3/c1-5(2-6,3-7)4-8/h2-4H2,1H3
InchiKey:	BYXOMFFBGDPXHB-UHFFFAOYSA-N
Formula:	C5H9Cl3O
SMILES:	CC(CCl)(CCl)CCl
Mol. weight [g/mol]:	191.48
CAS:	1067-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-41.73	kJ/mol	Joback Method
hf	-202.50	kJ/mol	Joback Method
hfus	13.88	kJ/mol	Joback Method
hvap	38.58	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.709		Crippen Method
mcvol	118.030	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	422.86	K	Joback Method
tc	624.33	K	Joback Method
tf	238.29	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.02	J/molxK	624.33	Joback Method
cpg	244.19	J/molxK	590.75	Joback Method
cpg	236.86	J/molxK	557.17	Joback Method
cpg	229.01	J/molxK	523.59	Joback Method
cpg	220.59	J/molxK	490.02	Joback Method
cpg	211.57	J/molxK	456.44	Joback Method
cpg	201.93	J/molxK	422.86	Joback Method
dvisc	0.0064698	Paxs	238.29	Joback Method

dvisc	0.0003883	Paxs	422.86	Joback Method
dvisc	0.0005164	Paxs	392.10	Joback Method
dvisc	0.0007207	Paxs	361.34	Joback Method
dvisc	0.0010703	Paxs	330.58	Joback Method
dvisc	0.0017240	Paxs	299.81	Joback Method
dvisc	0.0030966	Paxs	269.05	Joback Method
hfust	2.50	kJ/mol	291.30	NIST Webbook

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=C1067090&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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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