

Propanoic acid, 2,3-dichloro-, methyl ester

Other names:	Propionic acid, 2,3-dichloro-, methyl ester Methyl «alpha», «beta»-dichloropropionate Methyl 2,3-dichloropropanoate Methyl 2,3-dichloropropionate 2,3-Dichloropropionic acid, methyl ester
Inchi:	InChI=1S/C4H6Cl2O2/c1-8-4(7)3(6)2-5/h3H,2H2,1H3
InchiKey:	OFHMODDLBXETIK-UHFFFAOYSA-N
Formula:	C4H6Cl2O2
SMILES:	COC(=O)C(Cl)CCl
Mol. weight [g/mol]:	157.00
CAS:	3674-09-7

Physical Properties

Property code	Value	Unit	Source
gf	-277.42	kJ/mol	Joback Method
hf	-407.45	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	42.04	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	1.006		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	927.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	924.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1491.00		NIST Webbook
tb	441.63	K	Joback Method
tc	640.84	K	Joback Method
tf	251.84	K	Joback Method
vc	0.376	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.11	J/molxK	441.63	Joback Method
cpg	203.72	J/molxK	607.64	Joback Method
cpg	197.95	J/molxK	574.44	Joback Method
cpg	191.90	J/molxK	541.23	Joback Method
cpg	185.57	J/molxK	508.03	Joback Method
cpg	178.98	J/molxK	474.83	Joback Method
cpg	209.22	J/molxK	640.84	Joback Method
dvisc	0.0003390	Paxs	441.63	Joback Method
dvisc	0.0004356	Paxs	410.00	Joback Method
dvisc	0.0005838	Paxs	378.37	Joback Method
dvisc	0.0008253	Paxs	346.74	Joback Method
dvisc	0.0012506	Paxs	315.10	Joback Method
dvisc	0.0020794	Paxs	283.47	Joback Method
dvisc	0.0039286	Paxs	251.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.20	K	6.70	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=C3674097&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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