2,3-Dichloropropionyl chloride

Other names:	Propanoyl chloride, 2,3-dichloro-
	2,3-Dichloropropanoyl chloride
Inchi:	InChI=1S/C3H3Cl3O/c4-1-2(5)3(6)7/h2H,1H2
InchiKey:	JQELECXPPAOSTM-UHFFFAOYSA-N
Formula:	C3H3Cl3O
SMILES:	O=C(Cl)C(Cl)CCl
Mol. weight [g/mol]:	161.41
CAS:	7623-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-192.77	kJ/mol	Joback Method
hf	-270.33	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	41.78	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.598		Crippen Method
mcvol	91.420	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
rinpol	905.00		NIST Webbook
tb	433.76	K	Joback Method
tc	643.42	K	Joback Method
tf	248.26	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.64	J/mol×K	433.76	Joback Method
cpg	160.13	J/mol×K	608.48	Joback Method
cpg	156.20	J/mol×K	573.53	Joback Method
cpg	152.00	J/mol×K	538.59	Joback Method
cpg	147.52	J/mol×K	503.65	Joback Method
cpg	142.73	J/mol×K	468.70	Joback Method

cpg	163.78	J/mol×K	643.42	Joback Method
dvisc	0.0004459	Pa×s	433.76	Joback Method
dvisc	0.0005703	Pa×s	402.84	Joback Method
dvisc	0.0007599	Pa×s	371.93	Joback Method
dvisc	0.0010666	Pa×s	341.01	Joback Method
dvisc	0.0016018	Pa×s	310.09	Joback Method
dvisc	0.0026323	Pa×s	279.18	Joback Method
dvisc	0.0048954	Pa×s	248.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.70	K	2.30	NIST Webbook
tbrp	326.20	K	2.10	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C7623134&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume