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]: 161.42

Physical Properties

Property code	Value	Unit	Source
hf	-312.62	kJ/mol	Cheméo Relay (1.0)
hfus	14.19	kJ/mol	Joback Method
ie	10.80	eV	Cheméo Relay (1.0)
logp	1.598		Crippen Method
mcvol	91.420	ml/mol	McGowan Method
rinpol	905.00		NIST Webbook
rinpol	905.00		NIST Webbook
tb	427.59	K	Cheméo Relay (1.0)
tf	291.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.64	J/mol×K	433.76	Joback Method
cpg	142.73	J/mol×K	468.70	Joback Method
cpg	147.52	J/mol×K	503.65	Joback Method
cpg	152.00	J/mol×K	538.59	Joback Method
cpg	156.20	J/mol×K	573.53	Joback Method
cpg	160.13	J/mol×K	608.48	Joback Method
cpg	163.78	J/mol×K	643.42	Joback Method
dvisc	0.0048954	Pa×s	248.26	Joback Method
dvisc	0.0026323	Pa×s	279.18	Joback Method
dvisc	0.0016018	Pa×s	310.09	Joback Method
dvisc	0.0010666	Pa×s	341.01	Joback Method

dvisc	0.0007599	Pa×s	371.93	Joback Method
dvisc	0.0005703	Pa×s	402.84	Joback Method
dvisc	0.0004459	Pa×s	433.76	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: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7623134&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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