Propanoyl chloride, 3-chloro-

Other names:	3-Chloropropionyl chloride
	3-Chloropropionic acid chloride
	«beta»-Chloropropanoyl chloride
	«beta»-Chloropropionoyl chloride
	«beta»-Chloropropionyl chloride
	Propionyl chloride, 3-chloro-
	3-Chloropropanoyl chloride
	«beta»-Chloropropionic acid chloride
	NSC 84180
Inchi:	InChI=1S/C3H4Cl2O/c4-2-1-3(5)6/h1-2H2
InchiKey:	INUNLMUAPJVRME-UHFFFAOYSA-N
Formula:	C3H4Cl2O
SMILES:	O=C(Cl)CCCl
Mol. weight [g/mol]:	126.97
CAS:	625-36-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.40	kJ/mol	Joback Method
hf	-249.31	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	37.79	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.381		Crippen Method
mcvol	79.180	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
rinpol	841.90		NIST Webbook
rinpol	841.90		NIST Webbook
tb	417.20	K	NIST Webbook
tc	593.93	K	Joback Method
tf	233.34	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.84	J/mol×K	396.77	Joback Method
cpg	124.04	J/mol×K	429.63	Joback Method
cpg	128.97	J/mol×K	462.49	Joback Method
cpg	133.67	J/mol×K	495.35	Joback Method
cpg	138.11	J/mol×K	528.21	Joback Method
cpg	142.33	J/mol×K	561.07	Joback Method
cpg	146.32	J/mol×K	593.93	Joback Method
dvisc	0.0034494	Pa×s	233.34	Joback Method
dvisc	0.0020316	Pa×s	260.58	Joback Method
dvisc	0.0013226	Pa×s	287.82	Joback Method
dvisc	0.0009274	Pa×s	315.06	Joback Method
dvisc	0.0006881	Pa×s	342.29	Joback Method
dvisc	0.0005335	Pa×s	369.53	Joback Method
dvisc	0.0004283	Pa×s	396.77	Joback Method

Sources

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=C625365&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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