

2-chloropropionyl chloride

Other names:	Alpha-chloropropionyl chloride
Inchi:	InChI=1S/C3H4Cl2O/c1-2(4)3(5)6/h2H,1H3
InchiKey:	JEQDSBVHLKBEIZ-UHFFFAOYSA-N
Formula:	C3H4Cl2O
SMILES:	CC(Cl)C(=O)Cl
Mol. weight [g/mol]:	126.97
CAS:	7623-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-180.84	kJ/mol	Joback Method
hf	-254.59	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.379		Crippen Method
mcvol	79.180	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
rinpol	739.40		NIST Webbook
rinpol	739.40		NIST Webbook
tb	396.33	K	Joback Method
tc	598.36	K	Joback Method
tf	218.34	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.90	J/molxK	396.33	Joback Method
cpg	124.33	J/molxK	430.00	Joback Method
cpg	129.47	J/molxK	463.67	Joback Method
cpg	134.35	J/molxK	497.35	Joback Method
cpg	138.97	J/molxK	531.02	Joback Method
cpg	143.33	J/molxK	564.69	Joback Method

cpg	147.45	J/molxK	598.36	Joback Method
dvisc	0.0050802	Paxs	218.34	Joback Method
dvisc	0.0026045	Paxs	248.01	Joback Method
dvisc	0.0015401	Paxs	277.67	Joback Method
dvisc	0.0010079	Paxs	307.34	Joback Method
dvisc	0.0007108	Paxs	337.00	Joback Method
dvisc	0.0005304	Paxs	366.66	Joback Method
dvisc	0.0004135	Paxs	396.33	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=C7623098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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