Acetyl chloride, dichloro-

Other names:	2,2-Dichloroacetyl chloride
	ALPHA,ALPHA-DICHLORACETYL CHLORIDE
	Acetyl chloride, 2,2-dichloro-
	CHCl2COCl
	Chlorid kyseliny dichloroctove
	Chlorure de dichloracetyle
	DICHLOROACETIC ACID CHLORIDE
	Dichloracetyl chloride
	Dichloroacetyl chloride
	Dichloroethanoyl chloride
	UN 1765
	«alpha»,«alpha»-Dichloroacetyl chloride
	Â«alphaÂ»,Â«alphaÂ»-Dichloroacetyl chloride
Inchi:	InChI=1S/C2HCl3O/c3-1(4)2(5)6/h1H
InchiKey:	FBCCMZVIWNDFMO-UHFFFAOYSA-N
Formula:	C2HCl3O
SMILES:	O=C(Cl)C(Cl)Cl
Mol. weight [g/mol]:	147.39
CAS:	79-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-201.19	kJ/mol	Joback Method
hf	-241.00 ± 8.80	kJ/mol	NIST Webbook
hfl	-281.00 ± 8.40	kJ/mol	NIST Webbook
hfus	11.60	kJ/mol	Joback Method
hvap	39.56	kJ/mol	Joback Method
ie	11.00	eV	NIST Webbook
ie	11.27	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.556		Crippen Method
mcvol	77.330	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	4756.24	kPa	Joback Method
rinpol	726.00		NIST Webbook

tb	381.20 ± 1.00	K	NIST Webbook
tb	382.20	K	NIST Webbook
tb	380.70	K	NIST Webbook
tb	381.00 ± 3.00	K	NIST Webbook
tb	378.00 ± 3.00	K	NIST Webbook
tc	623.00	K	Joback Method
tf	236.99	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.37	J/mol×K	410.88	Joback Method
cpg	119.27	J/mol×K	587.65	Joback Method
cpg	116.71	J/mol×K	552.30	Joback Method
cpg	113.95	J/mol×K	516.94	Joback Method
cpg	110.98	J/mol×K	481.59	Joback Method
cpg	107.79	J/mol×K	446.23	Joback Method
cpg	121.64	J/mol×K	623.00	Joback Method
dvisc	0.0004723	Pa×s	410.88	Joback Method
dvisc	0.0006001	Pa×s	381.90	Joback Method
dvisc	0.0007931	Pa×s	352.92	Joback Method
dvisc	0.0011017	Pa×s	323.94	Joback Method
dvisc	0.0016327	Pa×s	294.95	Joback Method
dvisc	0.0026360	Pa×s	265.97	Joback Method
dvisc	0.0047850	Pa×s	236.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49951e+01
Coeff. B	-3.39864e+03
Coeff. C	-5.31770e+01
Temperature range (K), min.	284.26
Temperature range (K), max.	406.14

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1551.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79367&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor 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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