Acetyl chloride, trichloro-

Other names:	Acetyl chloride, 2,2,2-trichloro-
	CCl3COCl
	NSC 190466
	Superpalite
	Trichloroacetic acid chloride
	Trichloroacetochloride
	Trichloroacetyl chloride
	UN 2442
Inchi:	InChI=1S/C2Cl4O/c3-1(7)2(4,5)6
InchiKey:	PVFOMCVHYWHZJE-UHFFFAOYSA-N
Formula:	C2Cl4O
SMILES:	O=C(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	181.83
CAS:	76-02-8

Physical Properties

Property code	Value	Unit	Source
af	0.2345		Cheméo Relay (1.0)
gf	-207.84	kJ/mol	Joback Method
hf	-253.00	kJ/mol	NIST Webbook
hfl	-235.00 ± 8.40	kJ/mol	NIST Webbook
hfus	11.91	kJ/mol	Joback Method
hvap	39.76	kJ/mol	Cheméo Relay (1.0)
ie	11.31	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
logp	2.122		Crippen Method
mcvol	89.570	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
rinpol	778.00		NIST Webbook
rinpol	778.00		NIST Webbook
tb	391.00 ± 3.00	K	NIST Webbook
tb	391.20	K	NIST Webbook
tb	388.20	K	NIST Webbook
tc	633.87	K	Cheméo Relay (1.0)
tf	216.20 ± 0.10	K	NIST Webbook
vc	0.312	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.66	J/mol×K	636.65	Joback Method
cpg	139.32	J/mol×K	674.88	Joback Method
cpg	127.54	J/mol×K	483.75	Joback Method
cpg	130.67	J/mol×K	521.97	Joback Method
cpg	133.38	J/mol×K	560.20	Joback Method
cpg	135.70	J/mol×K	598.43	Joback Method
cpg	123.95	J/mol×K	445.52	Joback Method
dvisc	0.0017369	Pa×s	338.06	Joback Method
dvisc	0.0026611	Pa×s	311.19	Joback Method
dvisc	0.0044194	Pa×s	284.33	Joback Method
dvisc	0.0012071	Pa×s	364.92	Joback Method
dvisc	0.0008819	Pa×s	391.79	Joback Method
dvisc	0.0006708	Pa×s	418.65	Joback Method
dvisc	0.0005273	Pa×s	445.52	Joback Method
hvapt	38.30	kJ/mol	349.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46675e+01
Coeff. B	-3.42845e+03
Coeff. C	-4.99830e+01
Temperature range (K), min.	288.40
Temperature range (K), max.	416.43

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1769.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76028&Units=SI

Legend

af:	Acentric Factor
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
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