Trichloronitromethane

Other names:	Acquinite
	Chloorpikrine
	Chlor-o-pic
	Chloroform, nitro-
	Chloropicrin
	Chloropicrine
	Chlorpicrin
	Chlorpikrin
	Cloropicrina
	Dojyopicrin
	Dolochlor
	G 25
	KLOP
	Larvacide
	Larvacide 100
	Methane, trichloronitro-
	Microlysin
	NCI-C00533
	NSC 8743
	Nemax
	Nitrochloroform
	Nitromethane, 1,1,1-trichloro-
	Nitrotrichloromethane
	PS
	Pic-Clor
	Picfume
	Picride
	Profume A
	S 1
	Tri-Clor
	Trichloornitromethaan
	Trichlornitromethan
	Tricloro-nitro-metano
	UN 1580
Inchi:	InChI=1S/CCl3NO2/c2-1(3,4)5(6)7
InchiKey:	LFHISGNCFUNFFM-UHFFFAOYSA-N
Formula:	CCl3NO2
SMILES:	O=[N+]([O-])C(Cl)(Cl)Cl
Mol. weight [g/mol]:	164.38
CAS:	76-06-2

Physical Properties

Property code	Value	Unit	Source
gf	-39.86	kJ/mol	Joback Method
hf	-130.70	kJ/mol	Joback Method
hfus	14.88	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-2.00		Estimated Solubility Method
log10ws	-2.00		Aqueous Solubility Prediction Method
logp	1.591		Crippen Method
mcvol	79.090	ml/mol	McGowan Method
pc	5146.06	kPa	Joback Method
rinpol	761.00		NIST Webbook
tb	385.10 ± 0.70	K	NIST Webbook
tb	385.15 ± 1.50	K	NIST Webbook
tb	385.05 ± 0.50	K	NIST Webbook
tb	385.00 ± 0.50	K	NIST Webbook
tc	736.19	K	Joback Method
tf	206.55	K	Aqueous Solubility Prediction Method
tf	203.70 ± 0.02	K	NIST Webbook
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.68	J/mol×K	483.18	Joback Method
cpg	125.50	J/mol×K	525.35	Joback Method
cpg	128.77	J/mol×K	567.52	Joback Method
cpg	131.55	J/mol×K	609.68	Joback Method
cpg	133.89	J/mol×K	651.85	Joback Method
cpg	135.85	J/mol×K	694.02	Joback Method
cpg	137.47	J/mol×K	736.19	Joback Method
hvapt	39.30	kJ/mol	303.00	NIST Webbook
hvapt	38.50	kJ/mol	375.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76062&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
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