Trichloroacetyl isocyanate

Other names:	2,2,2-Trichloroacetyl isocyanate
	Acetyl isocyanate, trichloro-
Inchi:	InChI=1S/C3Cl3NO2/c4-3(5,6)2(9)7-1-8
InchiKey:	GRNOZCCBOFGDCL-UHFFFAOYSA-N
Formula:	C3Cl3NO2
SMILES:	O=C=NC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	188.40
CAS:	3019-71-4

Physical Properties

Property code	Value	Unit	Source
hf	-279.21	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	1.219		Crippen Method
mcvol	98.670	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	497.64	K	Joback Method
tc	727.14	K	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=C3019714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature