

Methane, chlorotrinitro-

Other names:	Chloronitroform Chlorotrinitromethane Trinitrochloromethane
Inchi:	InChI=1S/CCIN3O6/c2-1(3(6)7,4(8)9)5(10)11
InchiKey:	GNZCDDDPGSFZFG-UHFFFAOYSA-N
Formula:	CCIN3O6
SMILES:	O=[N+](O-)C(Cl)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	185.48
CAS:	1943-16-4

Physical Properties

Property code	Value	Unit	Source
gf	55.10	kJ/mol	Joback Method
hf	21.00	kJ/mol	NIST Webbook
hfl	-13.00	kJ/mol	NIST Webbook
hfl	-23.30 ± 0.75	kJ/mol	NIST Webbook
hfus	29.21	kJ/mol	Joback Method
hvap	45.44	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
log10ws	-2.24		Crippen Method
logp	-0.333		Crippen Method
mcvol	89.450	ml/mol	McGowan Method
pc	5953.74	kPa	Joback Method
tb	712.00	K	Joback Method
tc	1009.76	K	Joback Method
tf	278.90 ± 0.10	K	NIST Webbook
vc	0.376	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.57	J/mol×K	712.00	Joback Method
cpg	206.76	J/mol×K	761.63	Joback Method
cpg	210.27	J/mol×K	811.25	Joback Method

cpg	213.22	J/mol×K	860.88	Joback Method
cpg	215.70	J/mol×K	910.51	Joback Method
cpg	217.83	J/mol×K	960.14	Joback Method
cpg	219.70	J/mol×K	1009.76	Joback Method

Sources

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=C1943164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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