Benzene, 1,3,5-trichloro-2-nitro-

Other names:	1,3,5-Trichloro-2-nitrobenzene
	2,4,6-Trichloro-1-nitrobenzene
	2,4,6-Trichloronitrobenzene
	1-Nitro-2,4,6-trichlorobenzene
Inchi:	InChI=1S/C6H2Cl3NO2/c7-3-1-4(8)6(10(11)12)5(9)2-3/h1-2H
InchiKey:	AEBJDOTVYMITIA-UHFFFAOYSA-N
Formula:	C6H2Cl3NO2
SMILES:	O=[N+]([O-])c1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	226.44
CAS:	18708-70-8

Physical Properties

Property code	Value	Unit	Source
gf	82.92	kJ/mol	Joback Method
hf	-23.03	kJ/mol	Joback Method
hfus	28.12	kJ/mol	Joback Method
hsub	84.30 ± 1.90	kJ/mol	NIST Webbook
hsub	86.70 ± 1.10	kJ/mol	NIST Webbook
hvap	62.96	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.555		Crippen Method
mcvol	125.780	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	642.43	K	Joback Method
tc	910.67	K	Joback Method
tf	454.73	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.74	J/mol×K	642.43	Joback Method
cpg	240.49	J/mol×K	687.14	Joback Method
cpg	246.61	J/mol×K	731.84	Joback Method

cpg	252.16	J/mol×K	776.55	Joback Method
cpg	257.16	J/mol×K	821.25	Joback Method
cpg	261.64	J/mol×K	865.96	Joback Method
cpg	265.63	J/mol×K	910.67	Joback Method
hsubt	86.90 ± 1.10	kJ/mol	295.00	NIST Webbook

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=C18708708&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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