3,4,5-Trichloronitrobenzene

Other names: 3,4,5-Trichloronitrobenzene
1,2,3-trichloro-5-nitrobenzene
Inchi: InChI=1S/C6H2Cl3NO2/c7-4-1-3(10(11)12)2-5(8)6(4)9/h1-2H
InchiKey: HHLCSFGOTLUREE-UHFFFAOYSA-N
Formula: C6H2Cl3NO2
SMILES: O=[N+]([O-])c1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]: 226.45

Physical Properties

Property code	Value	Unit	Source
hf	-16.95	kJ/mol	Cheméo Relay (1.0)
hfus	28.12	kJ/mol	Joback Method
hvap	75.26	kJ/mol	Cheméo Relay (1.0)
ie	10.04	eV	Cheméo Relay (1.0)
log10ws	-4.31		Cheméo Relay (1.0)
logp	3.555		Crippen Method
mcvol	125.780	ml/mol	McGowan Method
tb	550.95	K	Cheméo Relay (1.0)
tf	393.25	K	Cheméo Relay (1.0)

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20098480&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point