2-Nitro-3,4,6-trichlorophenol

Other names: 2-Nitro-3,4,6-trichlorophenol
3,4,6-Trichloro-2-nitrophenol
Phenol, 3,4,6-trichloro-2-nitro-
Inchi: InChI=1S/C6H2Cl3NO3/c7-2-1-3(8)6(11)5(4(2)9)10(12)13/h1,11H
InchiKey: XWLBYVXDCGYXGY-UHFFFAOYSA-N
Formula: C6H2Cl3NO3
SMILES: O=[N+]([O-])c1c(O)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 242.45

Physical Properties

Property code	Value	Unit	Source
hfus	33.90	kJ/mol	Joback Method
log10ws	-3.93		Cheméo Relay (1.0)
logp	3.261		Crippen Method
mcvol	131.650	ml/mol	McGowan Method
tb	534.16	K	Cheméo Relay (1.0)
tf	365.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.61	J/mol×K	723.05	Joback Method
cpg	270.14	J/mol×K	768.84	Joback Method
cpg	275.31	J/mol×K	814.64	Joback Method
cpg	280.21	J/mol×K	860.43	Joback Method
cpg	284.96	J/mol×K	906.23	Joback Method
cpg	289.68	J/mol×K	952.02	Joback Method
cpg	294.46	J/mol×K	997.82	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82622&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
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