

Phenol, 2,4-dichloro-6-nitro-

Other names:	2,4-Dichloro-6-nitrophenol 2-Nitro-4,6-dichlorophenol 2,4-Dichlor-6-nitrofenol
Inchi:	InChI=1S/C6H3Cl2NO3/c7-3-1-4(8)6(10)5(2-3)9(11)12/h1-2,10H
InchiKey:	LYPMXMBQPXPNIQ-UHFFFAOYSA-N
Formula:	C6H3Cl2NO3
SMILES:	O=[N+](O)c1cc(Cl)cc(Cl)c1O
Mol. weight [g/mol]:	208.00
CAS:	609-89-2

Physical Properties

Property code	Value	Unit	Source
gf	-50.14	kJ/mol	Joback Method
hf	-173.13	kJ/mol	Joback Method
hfus	30.10	kJ/mol	Joback Method
hvap	70.92	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.607		Crippen Method
mcvol	119.410	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	680.64	K	Joback Method
tc	952.91	K	Joback Method
tf	524.01	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.14	J/molxK	680.64	Joback Method
cpg	257.55	J/molxK	726.02	Joback Method
cpg	263.45	J/molxK	771.40	Joback Method
cpg	268.94	J/molxK	816.77	Joback Method
cpg	274.16	J/molxK	862.15	Joback Method
cpg	279.21	J/molxK	907.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C609892&Units=SI

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
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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