2,6-Diiodo-4-nitrophenol

Other names:	Phenol, 2,6-diiodo-4-nitro-
	Ancylol
	Diisophenol
	Disofen
	DNP
	Disophenol
Inchi:	InChI=1S/C6H3I2NO3/c7-4-1-3(9(11)12)2-5(8)6(4)10/h1-2,10H
InchiKey:	UVGTXNPVQOQFQW-UHFFFAOYSA-N
Formula:	C6H3I2NO3
SMILES:	O=[N+]([O-])c1cc(I)c(O)c(I)c1
Mol. weight [g/mol]:	390.90
CAS:	305-85-1

Physical Properties

Property code	Value	Unit	Source
gf	89.96	kJ/mol	Joback Method
hf	12.09	kJ/mol	Joback Method
hfus	30.52	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.510		Crippen Method
mcvol	146.570	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	792.06	K	Joback Method
tc	1116.39	K	Joback Method
tf	580.29	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.77	J/mol×K	792.06	Joback Method
cpg	274.52	J/mol×K	846.11	Joback Method
cpg	280.18	J/mol×K	900.17	Joback Method

cpg	286.01	J/mol×K	954.22	Joback Method
cpg	292.25	J/mol×K	1008.28	Joback Method
cpg	299.17	J/mol×K	1062.33	Joback Method
cpg	307.02	J/mol×K	1116.39	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=C305851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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