

Nitroxinil

Other names:	Benzonitrile, 4-hydroxy-3-iodo-5-nitro-Dovenix 4-Hydroxy-3-iodo-5-nitrobenzonitrile Nitroxynil Trodax
Inchi:	InChI=1S/C7H3IN2O3/c8-5-1-4(3-9)2-6(7(5)11)10(12)13/h1-2,11H
InchiKey:	SGKGVABHDAQAJQ-UHFFFAOYSA-N
Formula:	C7H3IN2O3
SMILES:	N#Cc1cc(I)c(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	290.01
CAS:	1689-89-0

Physical Properties

Property code	Value	Unit	Source
gf	173.44	kJ/mol	Joback Method
hf	79.46	kJ/mol	Joback Method
hfus	30.21	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	1.777		Crippen Method
mcvol	136.220	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
rinpol	1754.00		NIST Webbook
tb	823.88	K	Joback Method
tc	1119.87	K	Joback Method
tf	598.49	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.19	J/mol×K	823.88	Joback Method
cpg	295.11	J/mol×K	873.21	Joback Method
cpg	300.91	J/mol×K	922.54	Joback Method

cpg	306.75	J/mol×K	971.87	Joback Method
cpg	312.80	J/mol×K	1021.20	Joback Method
cpg	319.23	J/mol×K	1070.53	Joback Method
cpg	326.22	J/mol×K	1119.87	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=C1689890&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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