

# Nitroxoline

<b>Other names:</b>	5-NOK 5-Nitro-8-hydroxyquinoline 5-Nitro-8-oxychinoline 5-Nitro-8-oxyquinoline 5-Nitro-quinolin-8-ol 5-Nitroks 5-Nitrox 5-Nitroxine 5-nitro-8-quinolinol 8-Quinolinol, 5-nitro- 8-hydroxy-5-nitroquinoline A-82 BAS 58 NSC 74947 Nibiol Nitroxolin Noxibiol Noxin Quinolin-8-ol, 5-nitro-
<b>Inchi:</b>	InChI=1S/C9H6N2O3/c12-8-4-3-7(11(13)14)6-2-1-5-10-9(6)8/h1-5,12H
<b>InchiKey:</b>	RJIWZDNTCBHXAL-UHFFFAOYSA-N
<b>Formula:</b>	C9H6N2O3
<b>SMILES:</b>	O=[N+](O)c1ccc(O)c2ncccc12
<b>Mol. weight [g/mol]:</b>	190.16
<b>CAS:</b>	4008-48-4

## Physical Properties

Property code	Value	Unit	Source
chs	-4283.40 ± 1.10	kJ/mol	NIST Webbook
hf	-1.70 ± 2.80	kJ/mol	NIST Webbook
hfs	-115.70 ± 1.70	kJ/mol	NIST Webbook
hsub	114.10 ± 2.20	kJ/mol	NIST Webbook
hsub	114.10 ± 2.20	kJ/mol	NIST Webbook
hsub	86.14	kJ/mol	NIST Webbook
hsub	111.20 ± 3.00	kJ/mol	NIST Webbook
log10ws	-3.24		Crippen Method
logp	1.849		Crippen Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.61	kJ/mol	455.20	NIST Webbook
hfust	24.70	kJ/mol	453.20	NIST Webbook
hsubt	81.66	kJ/mol	433.00	NIST Webbook
rhos	1489.70	kg/m <sup>3</sup>	298.15	Solubility determination and thermodynamic modeling of 5-nitro-8-hydroxyquinoline in ten organic solvents from T = (278.15 to 313.15) K and mixing properties of solutions

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Solubility determination and thermodynamic modeling of 5-nitro-8-hydroxyquinoline in ten organic solvents from T = (278.15 to 313.15) K and mixing properties of solutions: McGowan Method

<https://www.doi.org/10.1016/j.jct.2016.04.018>

<https://www.doi.org/10.1016/j.jct.2017.05.037>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4008484&Units=SI>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rhos:** Solid Density

Latest version available from:

<https://www.chemeo.com/cid/39-279-0/Nitroxoline.pdf>

Generated by Cheméo on 2024-04-25 19:16:33.180062216 +0000 UTC m=+16361842.100639528.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.