5-Amino-6-nitroquinoline

Other names:	5-Quinolinamine, 6-nitro-
	6-nitroquinolin-5-ylamine
Inchi:	InChI=1S/C9H7N3O2/c10-9-6-2-1-5-11-7(6)3-4-8(9)12(13)14/h1-5H,10H2
InchiKey:	TYBYHEXFKFLRFT-UHFFFAOYSA-N
Formula:	C9H7N3O2
SMILES:	Nc1c([N+](=O)[O-])ccc2ncccc12
Mol. weight [g/mol]:	189.17
CAS:	35975-00-9

Physical Properties

Property code	Value	Unit	Source
hsub	136.40 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.33		Crippen Method
logp	1.725		Crippen Method
mcvol	131.830	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	130.70 ± 0.80	kJ/mol	412.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35975009&Units=SI

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	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