

1H-Indole, 5-nitro-

Other names:	Indole, 5-nitro- 5-Nitroindole 5-Nitro-1H-indole
Inchi:	InChI=1S/C8H6N2O2/c11-10(12)7-1-2-8-6(5-7)3-4-9-8/h1-5,9H
InchiKey:	OZFPSOBLQZPIAV-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	O=[N+]([O-])c1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	162.15
CAS:	6146-52-7

Physical Properties

Property code	Value	Unit	Source
hsub	110.50 ± 1.00	kJ/mol	NIST Webbook
log10ws	-3.15		Crippen Method
logp	1.594		Crippen Method
mvol	112.060	ml/mol	McGowan Method

Sources

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=C6146527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

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