

7-Methyl 8-nitroquinoline

Other names:	Quinoline, 7-methyl-8-nitro- 8-Nitro-7-methylquinoline
Inchi:	InChI=1S/C10H8N2O2/c1-7-4-5-8-3-2-6-11-9(8)10(7)12(13)14/h2-6H,1H3
InchiKey:	ZZDTVYJYMRSNQL-UHFFFAOYSA-N
Formula:	C10H8N2O2
SMILES:	<chem>Cc1ccc2cccnc2c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	188.18
CAS:	7471-63-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	2.451		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
rinpol	305.75		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=C7471638&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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