5-nitro-8-methylquinoline

Inchi: InChI=1S/C10H8N2O2/c1-7-4-5-9(12(13)14)10-8(7)3-2-6-11-10/h2-6H,1H3
InchiKey: PJUFTRGYNSXIDE-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: Cc1ccc([N+](=O)[O-])c2ncccc12
Mol. weight [g/mol]: 188.18

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	288.56		NIST Webbook
rinpol	285.19		NIST Webbook
rinpol	288.52		NIST Webbook
rinpol	287.84		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=R151347&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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