2-Methyl-6-nitroquinoline

Other names: Quinoline, 2-methyl-6-nitro-
Inchi: InChI=1S/C10H8N2O2/c1-7-2-3-8-6-9(12(13)14)4-5-10(8)11-7/h2-6H,1H3
InchiKey: DXDPHHQJZWWAEH-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: Cc1ccc2cc([N+](=O)[O-])ccc2n1
Mol. weight [g/mol]: 188.18
CAS: 613-30-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	2.451		Crippen Method
mcvol	135.940	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=C613309&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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