5,6-Dimethoxy-8-nitro-quinoline

Inchi: InChI=1S/C11H10N2O4/c1-16-9-6-8(13(14)15)10-7(11(9)17-2)4-3-5-12-10/h3-6H,1-2H3
InchiKey: HDOJSHDBNBHDIM-UHFFFAOYSA-N
Formula: C11H10N2O4
SMILES: COc1cc([N+](=O)[O-])c2ncccc2c1OC
Mol. weight [g/mol]: 234.21
CAS: 5333-02-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.160		Crippen Method
mcvol	161.770	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5333028&Units=SI
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

Legend

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