4'-Nitroflavone

Inchi:	InChI=1S/C15H9NO4/c17-13-9-15(20-14-4-2-1-3-12(13)14)10-5-7-11(8-6-10)16(18)19/h1
InchiKey:	CKSVYVHLZNMXLX-UHFFFAOYSA-N
Formula:	C15H9NO4
SMILES:	O=c1cc(-c2ccc([N+](=O)[O-])cc2)oc2ccccc12
Mol. weight [g/mol]:	267.24
CAS:	19725-49-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.69		Crippen Method
logp	3.368		Crippen Method
mcvol	184.390	ml/mol	McGowan Method

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=C19725496&Units=SI

Legend

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

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