8-Hydroxy-7-iodo-5-quinoline sulfonic acid

Other names:	8-hydroxy-7-iodoquinoline-5-sulfonic acid
	8-hydroxy-7-iodoquinoline-5-sulphonic acid
Inchi:	InChI=1S/C9H6INO4S/c10-6-4-7(16(13,14)15)5-2-1-3-11-8(5)9(6)12/h1-4,12H,(H,13,14,1
InchiKey:	ZBJWWKFMHOAPNS-UHFFFAOYSA-N
Formula:	C9H6INO4S
SMILES:	O=S(=O)(O)c1cc(I)c(O)c2ncccc12
Mol. weight [g/mol]:	351.12
CAS:	547-91-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Aqueous Solubility Prediction Method
logp	1.792		Crippen Method
mcvol	170.080	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C547911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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

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