

5-Quinolinesulfonic acid, 8-hydroxy-7-(6-sulfo-2-naphthylazo)-

Inchi:	InChI=1S/C19H13N3O7S2/c23-19-16(10-17(31(27,28)29)15-2-1-7-20-18(15)19)22-21-13
InchiKey:	XGMFVZOKHBRUTL-QURGRASLSA-N
Formula:	C19H13N3O7S2
SMILES:	O=S(=O)(O)c1ccc2cc(N=Nc3cc(S(=O)(=O)O)c4cccnc4c3O)ccc2c1
Mol. weight [g/mol]:	459.45
CAS:	56990-57-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	4.002		Crippen Method
mcvol	291.560	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=C56990579&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

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