

8-HYDROXY-5-QUINOLINESULFONIC ACID

Other names:	5-Quinolinesulfonic acid, 8-hydroxy- Oxine-5-sulfonic acid 5-Sulfo-8-hydroxyquinoline 5-Sulfo-8-quinolinol 5-Sulfooxine 8-Hydroxy-5-quinolinesulfonic acid 8-Hydroxy-5-sulfoquinoline 8-Hydroxyquinoline-5-sulfonate 8-Hydroxyquinoline-5-sulphonic acid 8-Quinolinol-5-sulfonic acid Sulfoxine 8-Oxyquinoline-5-sulfonic acid NSC 13139
Inchi:	InChI=1S/C9H7NO4S/c11-7-3-4-8(15(12,13)14)6-2-1-5-10-9(6)7/h1-5,11H,(H,12,13,14)
InchiKey:	LGDFHDKSYGVKDC-UHFFFAOYSA-N
Formula:	C9H7NO4S
SMILES:	O=S(=O)(O)c1ccc(O)c2ncccc12
Mol. weight [g/mol]:	225.23

Physical Properties

Property code	Value	Unit	Source
hf	-489.52	kJ/mol	Cheméo Relay (1.0)
log10ws	-0.94		Cheméo Relay (1.0)
logp	1.187		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
tf	505.70	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C84888&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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