

2,2'-Dithiodipyridine-1,1'-dioxide

Inchi: InChI=1S/C10H8N2O2S2/c13-11-6-3-4-9(8-11)15-16-10-5-1-2-7-12(10)14/h1-8H
InchiKey: RISGLMSGXXNMHZ-UHFFFAOYSA-N
Formula: C10H8N2O2S2
SMILES: [O-][n+]1cccc(SSc2cccc[n+]2[O-])c1
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.82		Crippen Method
logp	1.753		Crippen Method
mcvol	168.640	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=B6003848&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/25-158-9/2-2-Dithiodipyridine-1-1-dioxide.pdf>

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