

6-Oxa-12-thia-indeno[1,2-b]fluorene

Inchi: InChI=1S/C18H10OS/c1-3-7-15-11(5-1)13-10-18-14(9-16(13)19-15)12-6-2-4-8-17(12)20
InchiKey: BTZKYJGIFCHEAR-UHFFFAOYSA-N
Formula: C18H10OS
SMILES: c1ccc2c(c1)oc1cc3c(cc12)sc1ccccc13
Mol. weight [g/mol]: 274.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.18		Crippen Method
logp	5.954		Crippen Method
mcvol	193.700	ml/mol	McGowan Method
rinpol	445.09		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R556519&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
rinpol: Non-polar retention indices

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