

«alpha»-Tertiophene

Inchi: InChI=1S/C14H12O3S2/c1-10(15)17-9-11(16)4-5-12-6-7-14(19-12)13-3-2-8-18-13/h2-3,6
InchiKey: PNRXZPUOVXRYEX-UHFFFAOYSA-N
Formula: C14H12O3S2
SMILES: CC(=O)OCC(O)C#Cc1ccc(-c2cccs2)s1
Mol. weight [g/mol]: 292.37
CAS: 95910-62-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.752		Crippen Method
mcvol	206.610	ml/mol	McGowan Method
rinpol	2527.20		NIST Webbook
rinpol	2527.20		NIST Webbook

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=C95910626&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/92-771-4/alpha-Tertiophene.pdf>

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