

Tiaprofenic acid, bis-methylated

Inchi: InChI=1S/C15H14O3S/c1-10(15(17)18-2)12-8-9-13(19-12)14(16)11-6-4-3-5-7-11/h3-10H
InchiKey: LUVJXUXGNTWIHI-UHFFFAOYSA-N
Formula: C15H14O3S
SMILES: COC(=O)C(C)c1ccc(C(=O)c2ccccc2)s1
Mol. weight [g/mol]: 274.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	3.256		Crippen Method
mcvol	204.350	ml/mol	McGowan Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		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=R201853&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

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<https://www.chemeo.com/cid/46-144-1/Tiaprofenic-acid-bis-methylated.pdf>

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