

4-Hydroxycoumarin, trifluoroacetate

Inchi: InChI=1S/C11H5F3O4/c12-11(13,14)10(16)18-8-5-9(15)17-7-4-2-1-3-6(7)8/h1-5H
InchiKey: RUUCIMGQPKJVHZ-UHFFFAOYSA-N
Formula: C11H5F3O4
SMILES: O=C(Oc1cc(=O)oc2ccccc12)C(F)(F)F
Mol. weight [g/mol]: 258.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.41		Crippen Method
logp	2.261		Crippen Method
mcvol	147.120	ml/mol	McGowan Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		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=U375583&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/79-862-8/4-Hydroxycoumarin-trifluoroacetate.pdf>

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