6-Methoxycoumarin

Inchi: InChI=1S/C10H8O3/c1-12-8-3-4-9-7(6-8)2-5-10(11)13-9/h2-6H,1H3
InchiKey: VKVCJIMMVPXDQD-UHFFFAOYSA-N
Formula: C10H8O3
SMILES: COc1ccc2oc(=O)ccc2c1
Mol. weight [g/mol]: 176.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.55		Crippen Method
logp	1.802		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
rinpol	1762.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1762.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R274272&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices