

7-Acetocoumarin

Inchi: InChI=1S/C11H8O3/c1-7(12)9-3-2-8-4-5-11(13)14-10(8)6-9/h2-6H,1H3
InchiKey: RBGLULORZMUTRO-UHFFFAOYSA-N
Formula: C11H8O3
SMILES: CC(=O)c1ccc2ccc(=O)oc2c1
Mol. weight [g/mol]: 188.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	1.996		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
rinpol	1779.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1779.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R274287&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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