6-Acetocoumarin

Inchi: InChI=1S/C11H8O3/c1-7(12)8-2-4-10-9(6-8)3-5-11(13)14-10/h2-6H,1H3
InchiKey: VIRDLAZXNXERGG-UHFFFAOYSA-N
Formula: C11H8O3
SMILES: CC(=O)c1ccc2oc(=O)ccc2c1
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	1768.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1768.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R274227&Units=SI
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

Legend

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