3-Acetylcoumarin

Other names: 2H-1-Benzopyran-2-one, 3-acetyl-
Coumarin, 3-acetyl-
3-Acetylcoumarine
Inchi: InChI=1S/C11H8O3/c1-7(12)9-6-8-4-2-3-5-10(8)14-11(9)13/h2-6H,1H3
InchiKey: CSPIFKKOBWYOEX-UHFFFAOYSA-N
Formula: C11H8O3
SMILES: CC(=O)c1cc2ccccc2oc1=O
Mol. weight [g/mol]: 188.18
CAS: 3949-36-8

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	1718.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3949368&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