

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

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