

4-Ethoxycoumarin

Inchi:	InChI=1S/C11H10O3/c1-2-13-10-7-11(12)14-9-6-4-3-5-8(9)10/h3-7H,2H2,1H3
InchiKey:	FLZDKBHAUILYAZ-UHFFFAOYSA-N
Formula:	C11H10O3
SMILES:	CCOc1cc(=O)oc2ccccc12
Mol. weight [g/mol]:	190.20
CAS:	35817-27-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.97		Crippen Method
logp	2.192		Crippen Method
mcvol	140.240	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C35817277&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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