

Ethyl 3-coumarincarboxylate

Other names:	Coumarin-3-carboxylic acid ethyl ester Ethyl coumarin-3-carboxylate 2H-1-Benzopyran-3-carboxylic acid, 2-oxo-, ethyl ester 1,2-Benzopyran-2-one-3-carboxylic acid, ethyl ester 3-Carbethoxycoumarin 3-Ethoxycarbonylcoumarin
Inchi:	InChI=1S/C12H10O4/c1-2-15-11(13)9-7-8-5-3-4-6-10(8)16-12(9)14/h3-7H,2H2,1H3
InchiKey:	XKHPEMKBJGUYCM-UHFFFAOYSA-N
Formula:	C12H10O4
SMILES:	CCOC(=O)c1cc2ccccc2oc1=O
Mol. weight [g/mol]:	218.21
CAS:	1846-76-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	1.970		Crippen Method
mcvol	155.900	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1846760&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

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