

Acetic acid, (3-ethyl-4-methyl-7-coumarinyloxy)-, ethyl ester

InChI:	InChI=1S/C16H18O5/c1-4-12-10(3)13-7-6-11(8-14(13)21-16(12)18)20-9-15(17)19-5-2/h
InChIKey:	QQULBZLVGXDJBG-UHFFFAOYSA-N
Formula:	C16H18O5
SMILES:	CCOC(=O)COc1ccc2c(C)c(CC)c(=O)oc2c1
Mol. weight [g/mol]:	290.31
CAS:	116373-43-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	2.606		Crippen Method
mcvol	218.130	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373434&Units=SI
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

Legend

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

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