

ethyl biscoumacetate

Inchi:	InChI=1S/C22H16O8/c1-2-28-20(25)15(16-18(23)11-7-3-5-9-13(11)29-21(16)26)17-19(2
InchiKey:	JCLHQQFUTFHUXNN-UHFFFAOYSA-N
Formula:	C22H16O8
SMILES:	CCOC(=O)C(c1c(O)c2cccc2oc1=O)c1c(O)c2cccc2oc1=O
Mol. weight [g/mol]:	408.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Aqueous Solubility Prediction Method
logp	3.006		Crippen Method
mcvol	277.060	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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

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