

Acetic acid, [(3,4-dimethyl-2-oxo-2h-1-benzopyran-7-yl)oxy]-, ethyl ester

InChI: InChI=1S/C15H16O5/c1-4-18-14(16)8-19-11-5-6-12-9(2)10(3)15(17)20-13(12)7-11/h5-7H
InChIKey: IKDRPWUBFBORSQ-UHFFFAOYSA-N
Formula: C15H16O5
SMILES: CCOC(=O)COc1ccc2c(C)c(C)c(=O)oc2c1
Mol. weight [g/mol]: 276.28
CAS: 35679-90-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.62		Crippen Method
logp	2.352		Crippen Method
mvol	204.040	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C35679904&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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