

Furan-3-carboxylic acid, 4-methyl-2-(2-methoxycarbonylethyl)-5-(4-oxopen-2-yl)methyl ester

InChI: InChI=1S/C16H22O6/c1-10(17)6-5-7-12-11(2)15(16(19)21-4)13(22-12)8-9-14(18)20-3/h5

InChIKey: FXPPITHUWLKGN-UHFFFAOYSA-N

Formula: C16H22O6

SMILES: COC(=O)CCc1oc(CCCC(C)=O)c(C)c1C(=O)OC

Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.76		Crippen Method
logp	2.392		Crippen Method
mcvol	239.160	ml/mol	McGowan Method
rinpole	2100.00		NIST Webbook
rinpole	2100.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R106535&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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