

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

Inchi: InChI=1S/C16H24O6/c1-10(17)6-5-7-12-11(2)15(16(19)21-4)13(22-12)8-9-14(18)20-3/h1-10,12-14,16-18,20-21,23-24
InchiKey: DXNPICWTUYIJFL-UHFFFAOYSA-N

Formula: C₁₆H₂₄O₆
SMILES: COC(=O)CCc1oc(CCCC(C)O)c(C)c1C(=O)OC
Mol. weight [g/mol]: 312.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	2.184		Crippen Method
mcvol	243.460	ml/mol	McGowan Method
rinpole	2119.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R106520&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpole: Non-polar retention indices

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