

3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid, dimethyl ester

Other names: Furan-3-carboxylic acid, 4-methyl-2-(2-methoxycarbonylethyl)-5-propyl, methyl ester
Inchi: InChI=1S/C14H20O5/c1-5-6-10-9(2)13(14(16)18-4)11(19-10)7-8-12(15)17-3/h5-8H2,1-4H1
InchiKey: MFHNAPOFQOZYAR-UHFFFAOYSA-N
Formula: C14H20O5
SMILES: CCCc1oc(CCC(=O)OC)c(C(=O)OC)c1C
Mol. weight [g/mol]: 268.31
CAS: 72719-10-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.65		Crippen Method
logp	2.433		Crippen Method
mcvol	209.410	ml/mol	McGowan Method
rinsol	1938.00		NIST Webbook
rinsol	1938.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C72719109&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
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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