

[7-(2-methylbut-2-enoyloxy)-5,6,7,8-tetrahydro-3H-2,3-dihydroxy-2-(1-methoxyethyl)-3-methylbutano

InChI=1S/C21H33NO7/c17-13(2)18(23)20-16-9-11-21-10-8-15(1)(16)22-12-29-19(24)2
InChIKey: QHOZSLCKHFUSU-UHFFFAOYSA-N

Formula: C21H33NO7

SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)OC)C(C)(C)O)C12

Mol. weight [g/mol]: 411.49

CAS: 303-34-4

Physical Properties

Property code	Value	Unit	Source
logp	0.959		Crippen Method
mcvol	318.900	ml/mol	McGowan Method
tf	368.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

Latest version available from:

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