

[6-[6-[[4-acetyloxy-10-hydroxy-5-methoxy-9,16-dimethylbutanoate

InChI: InChI=1S/C42H69NO15/c1-23(2)19-32(47)56-40-27(6)53-34(22-42(40,8)50)57-37-26(5)51-33-31-35-36-38-39-41-43-44-45-46-48-49-52-54-55-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/h1-42,44-46,48-50,52-54,56-58,60-62,64-66,68-70,72-74,76-78,80-82,84-86,88-90,92-94,96-98,100/t43-45,47-49,51-53,55-57,59-61,63-65,67-69,71-73,75-77,79-81,83-85,87-89,91-93,95-97,99-101/m1/s1

InchiKey: XJSFLOJWULLJQS-UHFFFAOYSA-N

Formula: C42H69NO15

SMILES: COC1C(OC(C)=O)CC(=O)OC(C)CC=CC=CC(O)C(C)CC(CC=O)C1OC1OC(C)C(OC2CC(C)C(C)C2)OC2C(C)C(C)C2

Mol. weight [g/mol]: 828.01

CAS: 16846-24-5

Physical Properties

Property code	Value	Unit	Source
hfus	119.99	kJ/mol	Joback Method
logp	3.013		Crippen Method
mcvol	642.290	ml/mol	McGowan Method
tf	404.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.80280e+01
Coeff. B	3.96522e+00
Coeff. C	-1.47516e-03
Coeff. D	-7.09000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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