

10-(3-carboxypropanoyloxy)-2,4a,6a,6b,9,9,12a-hexahydro-1H-benzocyclopenta[1,2-b:4,5-b']dipyrrolo[3,2-d:2',3'-d']pyrrole-5-carboxylic acid

InChI=1S/C34H50O7/c1-29(2)23-10-13-34(7)27(32(23,5)12-11-24(29)41-26(38)9-8-25(3)33-31-30-32)/p1/s1
InChIKey: OBZHEBDUNPOCJG-UHFFFAOYSA-N
Formula: C34H50O7
SMILES: CC1(C(=O)O)CCC2(C)CCC3(C)C(=CC(=O)C4C5(C)CCC(OC(=O)CCC(=O)O)C(C)(C)C5=CC=C4)C3=CC=C21
Mol. weight [g/mol]: 570.77
CAS: 5697-56-3

Physical Properties

Property code	Value	Unit	Source
hfus	52.36	kJ/mol	Joback Method
logp	6.828		Crippen Method
mcvol	455.210	ml/mol	McGowan Method
tf	565.65	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	-4.92208e+02
Coeff. B	5.30314e+00
Coeff. C	-5.24744e-03
Coeff. D	2.19280e-06
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

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

Crippen Method:

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

Crippen Method:

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

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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