Vincaleukoblastine

Inchi: InChI=1S/C46H58N4O9/c1-8-42(54)23-28-24-45(40(52)57-6,36-30(15-19-49(25-28)26-4
InchiKey: JXLYSJRDGCGARV-UHFFFAOYSA-N
Formula: C46H58N4O9
SMILES: CCC1(O)CC2CN(CCc3c([nH]c4ccccc34)C(C(=O)OC)(c3cc4c(cc3OC)N(C)C3C(O)(C(=O
Mol. weight [g/mol]: 810.99
CAS: 865-21-4

Physical Properties

Property code	Value	Unit	Source
logp	3.509		Crippen Method
mcvol	606.710	ml/mol	McGowan Method
tf	513.40	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/110-120-5/Vincaleukoblastine.pdf

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