

Cisapride

Inchi:	InChI=1S/C23H29ClFN3O4/c1-30-21-13-19(26)18(24)12-17(21)23(29)27-20-8-10-28(14)
InchiKey:	DCSUBABJRZXOMT-UHFFFAOYSA-N
Formula:	C23H29ClFN3O4
SMILES:	<chem>COc1cc(N)c(Cl)cc1C(=O)NC1CCN(CCCOc2ccc(F)cc2)CC1OC</chem>
Mol. weight [g/mol]:	465.95
CAS:	81098-60-4

Physical Properties

Property code	Value	Unit	Source
logp	3.358		Crippen Method
mcvol	339.680	ml/mol	McGowan Method
tf	383.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

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

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

<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

Cheméo Relay (1.0):

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/101-046-8/Cisapride.pdf>

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