

Ifenprodil

Inchi:	InChI=1S/C21H27NO2/c1-16(21(24)19-7-9-20(23)10-8-19)22-13-11-18(12-14-22)15-17-5
InchiKey:	UYNVMODNBIQBMV-UHFFFAOYSA-N
Formula:	C21H27NO2
SMILES:	CC(C(O)c1ccc(O)cc1)N1CCC(Cc2ccccc2)CC1
Mol. weight [g/mol]:	325.45
CAS:	23210-56-2

Physical Properties

Property code	Value	Unit	Source
logp	3.769		Crippen Method
mcvol	270.090	ml/mol	McGowan Method
tb	691.88	K	Cheméo Relay (1.0)
tf	387.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

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<https://www.chemeo.com/cid/101-529-2/lfenprodil.pdf>

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