

Oxaprozin

Inchi:	InChI=1S/C18H15NO3/c20-16(21)12-11-15-19-17(13-7-3-1-4-8-13)18(22-15)14-9-5-2-6-
InchiKey:	OFPXSFXSNFPTHF-UHFFFAOYSA-N
Formula:	C18H15NO3
SMILES:	O=C(O)CCc1nc(-c2ccccc2)c(-c2ccccc2)o1
Mol. weight [g/mol]:	293.32
CAS:	21256-18-8

Physical Properties

Property code	Value	Unit	Source
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-3.97		Cheméo Relay (1.0)
logp	4.026		Crippen Method
mcvol	220.790	ml/mol	McGowan Method
pc	2683.86	kPa	Cheméo Relay (1.0, beta)
tb	692.66	K	Cheméo Relay (1.0)
tf	433.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):	
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

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

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

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