Debrisoquine

Inchi: InChI=1S/C10H13N3/c11-10(12)13-6-5-8-3-1-2-4-9(8)7-13/h1-4H,5-7H2,(H3,11,12)
InchiKey: JWPGJSVJDAJRLW-UHFFFAOYSA-N
Formula: C10H13N3
SMILES: N=C(N)N1CCc2ccccc2C1
Mol. weight [g/mol]: 175.24
CAS: 1131-64-2

Physical Properties

Property code	Value	Unit	Source
logp	0.938		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
tf	552.15	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_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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/100-477-1/Debrisoquine.pdf

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