

Dimezone S

Inchi:	InChI=1S/C11H14N2O2/c1-11(8-14)7-13(12-10(11)15)9-5-3-2-4-6-9/h2-6,14H,7-8H2,1H3
InchiKey:	DSVIHYOAKPVFEH-UHFFFAOYSA-N
Formula:	C11H14N2O2
SMILES:	CC1(CO)CN(c2ccccc2)NC1=O
Mol. weight [g/mol]:	206.25
CAS:	13047-13-7

Physical Properties

Property code	Value	Unit	Source
logp	0.536		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
tf	398.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0):

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

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/106-526-0/Dimezone-S.pdf>

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