

MeIQ

Inchi:	InChI=1S/C12H12N4/c1-7-6-9-8(4-3-5-14-9)10-11(7)16(2)12(13)15-10/h3-6H,1-2H3,(H2,
InchiKey:	GMGWMIJIGUYNAY-UHFFFAOYSA-N
Formula:	C12H12N4
SMILES:	Cc1cc2ncccc2c2nc(N)n(C)c12
Mol. weight [g/mol]:	212.26
CAS:	77094-11-2

Physical Properties

Property code	Value	Unit	Source
logp	2.012		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
tf	570.15	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

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<https://www.chemeo.com/cid/108-744-6/MeIQ.pdf>

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