

PROTHIONAMIDE

Inchi: InChI=1S/C9H12N2S/c1-2-3-8-6-7(9(10)12)4-5-11-8/h4-6H,2-3H2,1H3,(H2,10,12)
InchiKey: VRDIULHPQTYCLN-UHFFFAOYSA-N
Formula: C9H12N2S
SMILES: CCCc1cc(C(N)=S)ccn1
Mol. weight [g/mol]: 180.28

Physical Properties

Property code	Value	Unit	Source
logp	1.668		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
tb	576.27	K	Cheméo Relay (1.0)
tf	416.85	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C14222607>

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.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/102-801-8/PROTHIONAMIDE.pdf>

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