DESMETHYLCOTININE

Inchi: InChI=1S/C9H10N2O/c12-9-4-3-8(11-9)7-2-1-5-10-6-7/h1-2,5-6,8H,3-4H2,(H,11,12)
InchiKey: FXFANIORDKRCCA-UHFFFAOYSA-N
Formula: C9H10N2O
SMILES: O=C1CCC(c2cccnc2)N1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
hvap	93.22	kJ/mol	Cheméo Relay (1.0)
log10ws	-0.28		Cheméo Relay (1.0)
logp	1.033		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
tb	596.40	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C17708871
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.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature