1-METHYL-3-PYRROLIDINOL

Other names: N-Methyl-3-pyrrolidinol
3-Pyrrolidinol, 1-methyl-
1-methylpyrrolidin-3-ol
Inchi: InChI=1S/C5H11NO/c1-6-3-2-5(7)4-6/h5,7H,2-4H2,1H3
InchiKey: FLVFPAIGVBQGET-UHFFFAOYSA-N
Formula: C5H11NO
SMILES: CN1CCC(O)C1
Mol. weight [g/mol]: 101.15

Physical Properties

Property code	Value	Unit	Source
hvap	69.65	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
logp	-0.317		Crippen Method
mcvol	86.300	ml/mol	McGowan Method
tb	430.36	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	324.20	K	0.10	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13220332&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure