

Pempidine

Other names:	1,2,2,6,6-Pentamethylpiperidine M&B 4486 M+B 4486 N-Methyl-2,2,6,6-Tetramethylpiperidine Perolysen Piperidine, 1,2,2,6,6-pentamethyl- Pyrilene Tenormal
Inchi:	InChI=1S/C10H21N/c1-9(2)7-6-8-10(3,4)11(9)5/h6-8H2,1-5H3
InchiKey:	XULIXFLCVXWHRF-UHFFFAOYSA-N
Formula:	C10H21N
SMILES:	CN1C(C)(C)CCCC1(C)C
Mol. weight [g/mol]:	155.28
CAS:	79-55-0

Physical Properties

Property code	Value	Unit	Source
ie	7.23 ± 0.05	eV	NIST Webbook
log10ws	-2.70		Crippen Method
logp	2.659		Crippen Method
mcvol	150.880	ml/mol	McGowan Method
tb	460.70	K	NIST Webbook
tb	420.20	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.17565e+01
Coeff. B	-2.87490e+03
Coeff. C	-5.79520e+01
Temperature range (K), min.	308.62
Temperature range (K), max.	504.01

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79550&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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