

N-Ethylpiperazine

Other names:	1-Ethyl-2,5-dihydropiperazine 1-Ethylpiperazine Piperazine, 1-ethyl-
Inchi:	InChI=1S/C6H14N2/c1-2-8-5-3-7-4-6-8/h7H,2-6H2,1H3
InchiKey:	WGCYRFWNGRMRJA-UHFFFAOYSA-N
Formula:	C6H14N2
SMILES:	CCN1CCNCC1
Mol. weight [g/mol]:	114.19
CAS:	5308-25-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.01		Crippen Method
logp	-0.088		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
ripol	944.00		NIST Webbook
ripol	936.00		NIST Webbook
ripol	934.00		NIST Webbook
ripol	970.00		NIST Webbook
ripol	944.00		NIST Webbook
ripol	970.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1370.00		NIST Webbook
tb	430.15 ± 2.00	K	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55490e+01
Coeff. B	-4.03799e+03
Coeff. C	-6.07320e+01
Temperature range (K), min.	325.32
Temperature range (K), max.	455.16

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=C5308258&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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