1-Ethylpiperazine

Other names:	1-Ethyl-2,5-dihydropiperazine
	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
hvap	54.09	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
logp	-0.088		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	936.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1332.00		NIST Webbook
tb	430.15 ± 2.00	K	NIST Webbook
tf	246.20	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5308258&Units=SI

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
ie: Ionization energy
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
tf: Normal melting (fusion) point