

1-(2-HYDROXYETHYL)PYRROLIDINE

Other names:	1-Pyrrolidineethanol
	2-(1-pyrrolidino)ethanol
	2-(1-pyrrolidiny)ethanol
	2-pyrrolidin-1-ylethanol
	HEP
	N-(2-Hydroxyethyl)pyrrolidine
	N-(2-hydroxyethyl)pyrrolidine
	Pyrrolidinoethanol
Inchi:	InChI=1S/C6H13NO/c8-6-5-7-3-1-2-4-7/h8H,1-6H2
InchiKey:	XBRDBODLCHKXHI-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	OCCN1CCCC1
Mol. weight [g/mol]:	115.18

Physical Properties

Property code	Value	Unit	Source
hvap	61.43	kJ/mol	Cheméo Relay (1.0)
logp	0.075		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
ripol	1552.00		NIST Webbook
ripol	1564.00	NIST Webbook	NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1552.00		NIST Webbook
tb	458.35	K	Cheméo Relay (1.0)
tf	260.68	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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tbp	360.60	K	2.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	372.20	K	4.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	388.80	K	9.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	405.50	K	19.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	417.00	K	29.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	426.10	K	39.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	432.60	K	49.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture

tbp	438.10	K	59.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	442.60	K	69.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	446.90	K	79.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	449.80	K	89.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbrp	353.20	K	1.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture:	https://www.doi.org/10.1016/j.jct.2019.06.017
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2955886&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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