N-«beta»-Hydroxyethylpyrrolidine

Other names:	1-(2-hydroxyethyl)pyrrolidine
	1-Pyrrolidineethanol
	2-(1-pyrrolidino)ethanol
	2-(1-pyrrolidinyl)ethanol
	2-pyrrolidin-1-ylethanol
	HEP
	N-(2-Hydroxethyl)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]:	115.17
CAS:	2955-88-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.06		Crippen Method
logp	0.075		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
ripol	1564.00		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1552.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

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	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	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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2955886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure