

N-(.beta.-Hydroxyethyl)hexamethyleneimine

Other names:	2-(n-Hexamethyleneimino)ethanol N-(«beta»-Hydroxyethyl)hexamethyleneimine 1H-Azepine-1-ethanol, hexahydro- Hexahydro-1H-azepine-1-ethanol N-(2-Hydroxyethyl)hexamethyleneimine 2-(1-azoniacyclohept-1-yl)ethanol 2-(azepan-1-yl)ethanol
Inchi:	InChI=1S/C8H17NO/c10-8-7-9-5-3-1-2-4-6-9/h10H,1-8H2
InchiKey:	VMRYMOMQCYSPPH-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	OCCN1CCCCC1
Mol. weight [g/mol]:	143.23

Physical Properties

Property code	Value	Unit	Source
hvap	67.52	kJ/mol	Cheméo Relay (1.0)
logp	0.855		Crippen Method
mcvol	128.570	ml/mol	McGowan Method
tb	498.60	K	Cheméo Relay (1.0)
tf	293.33	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20603003&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
t_b:	Normal Boiling Point Temperature
t_f:	Normal melting (fusion) point

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