

1,4-Bis(2-hydroxyethyl)piperazine

Other names:	N,N'-Bis(2-hydroxyethyl)piperazine di(N-Hydroxyethyl)piperazine 1,4-Piperazinediethanol N,N'-Bis(«beta»-hydroxyethyl)piperazine N,N'-Di(2-hydroxyethyl)piperazine N,N'-Dihydroxyethylpiperazine Piperazine, N,N'-bis(2-hydroxyethyl)- 1,4-Bis(«beta»-hydroxyethyl)piperazine 1,4-Di(2-hydroxyethyl)piperazine NSC 26892 NSC 36645 piperazine-1,4-diethanol
Inchi:	InChI=1S/C8H18N2O2/c11-7-5-9-1-2-10(4-3-9)6-8-12/h11-12H,1-8H2
InchiKey:	VARKIGWTYBUWNT-UHFFFAOYSA-N
Formula:	C8H18N2O2
SMILES:	OCCN1CCN(CCO)CC1
Mol. weight [g/mol]:	174.24
CAS:	122-96-3

Physical Properties

Property code	Value	Unit	Source
chs	-5256.50 ± 1.60	kJ/mol	NIST Webbook
hfs	-464.10 ± 1.50	kJ/mol	NIST Webbook
hsub	130.50 ± 1.00	kJ/mol	NIST Webbook
log10ws	1.27		Crippen Method
logp	-1.411		Crippen Method
mcvol	144.420	ml/mol	McGowan Method
tb	551.00	K	NIST Webbook
tf	405.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	250.68	J/mol×K	298.00	NIST Webbook

hfust	25.90	kJ/mol	405.00	NIST Webbook
hfust	25.90	kJ/mol	405.00	NIST Webbook
hsubt	104.10	kJ/mol	345.00	NIST Webbook
hsubt	128.00 ± 1.00	kJ/mol	375.00	NIST Webbook
hsubt	104.10 ± 4.60	kJ/mol	334.00	NIST Webbook
hvapt	67.80 ± 5.30	kJ/mol	460.00	NIST Webbook
sfust	64.00	J/mol×K	405.00	NIST Webbook

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=C122963&Units=SI>

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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