N,N-Bis[(hydroxyethyl)trimethylene]diamine

Other names:	Ethanol, 2,2'-[(3-aminopropyl)imino]bis- Aminopropyldiethanolamine Ethanol, 2,2'-(aminopropylimino)- Ethanol, 2,2'-((3-aminopropyl)imino)di- N-(3-Aminopropyl)diethanolamine N,N-Bis(hydroxyethyl)-1,3-propanediamine N,N-Bis(2-hydroxyethyl)-1,3-propanediamine N,N-Di(2-hydroxyethyl)-1,3-propanediamine 2,2'-((3-Aminopropyl)imino)diethanol (3-Aminopropyl)diethanolamine NSC 8172 N-(3-aminopropyl)iminodiethanol
Inchi:	InChI=1S/C7H18N2O2/c8-2-1-3-9(4-6-10)5-7-11/h10-11H,1-8H2
InchiKey:	FKJVYOFPTRGCSP-UHFFFAOYSA-N
Formula:	C7H18N2O2
SMILES:	NCCCN(CCO)CCO
Mol. weight [g/mol]:	162.23
CAS:	4985-85-7

Physical Properties

Property code	Value	Unit	Source
gf	-88.35	kJ/mol	Joback Method
hf	-390.95	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	0.72		Crippen Method
logp	-1.378		Crippen Method
mcvol	141.190	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	480.00	K	NIST Webbook
tc	795.11	K	Joback Method
tf	406.02	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.03	J/mol×K	628.89	Joback Method
cpg	400.96	J/mol×K	656.59	Joback Method
cpg	410.44	J/mol×K	684.30	Joback Method
cpg	419.48	J/mol×K	712.00	Joback Method
cpg	428.10	J/mol×K	739.70	Joback Method
cpg	436.31	J/mol×K	767.40	Joback Method
cpg	444.14	J/mol×K	795.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.50 ± 2.50	K	0.30	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4985857&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume