

trans-1,4-Bis(aminomethyl)cyclohexane

Other names:	1,4-Cyclohexanedimethanamine, trans- 1,4-Cyclohexanebis(methylamine), trans- 1,4-Cyclohexanedimethylamine, trans- trans-1,4-Cyclohexanebis(methylamine) [4-(Aminomethyl)cyclohexyl]methylamine, trans
Inchi:	InChI=1S/C8H18N2/c9-5-7-1-2-8(6-10)4-3-7/h7-8H,1-6,9-10H2/t7-,8-
InchiKey:	OXIKYYJDTWKERT-ZKCHVHJHSA-N
Formula:	C8H18N2
SMILES:	NCC1CCC(CN)CC1
Mol. weight [g/mol]:	142.24
CAS:	10029-07-9

Physical Properties

Property code	Value	Unit	Source
gf	166.12	kJ/mol	Joback Method
hf	-106.89	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	54.80	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	0.710		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	542.38	K	Joback Method
tc	767.39	K	Joback Method
tf	349.58	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.06	J/molxK	542.38	Joback Method
cpg	359.98	J/molxK	579.88	Joback Method
cpg	376.86	J/molxK	617.38	Joback Method
cpg	392.72	J/molxK	654.89	Joback Method

cpg	407.59	J/mol×K	692.39	Joback Method
cpg	421.50	J/mol×K	729.89	Joback Method
cpg	434.47	J/mol×K	767.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10029079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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