

1,3-Propanediamine, N,N'-bis(2-aminoethyl)-

Other names:	N,N'-Bis(2-aminoethyl)-1,3-propanediamine 1,4,8,11-Tetraazaundecane Ethylenetrimethyleneethylenetetramine N,N'-Bis(2-aminoethyl)propane-1,3-diamine 1,4,8,11-Tetrazaundecane 1,9-Diamino-3,7-diazanonane 3,7-Diazanonane-1,9-diamine
Inchi:	InChI=1S/C7H20N4/c8-2-6-10-4-1-5-11-7-3-9/h10-11H,1-9H2
InchiKey:	UWMHHZFHBCYGCV-UHFFFAOYSA-N
Formula:	C7H20N4
SMILES:	NCCNCCCNCN
Mol. weight [g/mol]:	160.26
CAS:	4741-99-5

Physical Properties

Property code	Value	Unit	Source
gf	319.74	kJ/mol	Joback Method
hf	-13.29	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	65.33	kJ/mol	Joback Method
log10ws	3.36e-04		Crippen Method
logp	-1.527		Crippen Method
mvol	149.410	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	604.96	K	Joback Method
tc	798.15	K	Joback Method
tf	440.49	K	Joback Method
vc	0.555	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.24	J/mol×K	765.95	Joback Method
cpg	406.26	J/mol×K	604.96	Joback Method

cpg	419.34	J/mol×K	637.16	Joback Method
cpg	431.76	J/mol×K	669.36	Joback Method
cpg	443.53	J/mol×K	701.56	Joback Method
cpg	454.68	J/mol×K	733.75	Joback Method
cpg	475.22	J/mol×K	798.15	Joback Method
hvapt	98.30 ± 1.30	kJ/mol	340.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.70	K	1.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4741995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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

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