

1,3-Propanediamine, N,N-dibutyl-

Other names:	N,N-Dibutyl-1,3-propanediamine N,N-Dibutylaminopropylamine N,N-Dibutyltrimethylenediamine 3-(Dibutylamino)propylamine 3-(di-Normal-butylamino)-propylamine 3-(Dibutylamino)-n-propylamine N,N-di-n-Butyl-1,3-propanediamine 1,3-Propanediamine, N1,N1-dibutyl- NSC 6333 3-aminopropyldibutylamine
Inchi:	InChI=1S/C11H26N2/c1-3-5-9-13(10-6-4-2)11-7-8-12/h3-12H2,1-2H3
InchiKey:	KYCGURZGBKFEQB-UHFFFAOYSA-N
Formula:	C11H26N2
SMILES:	CCCCN(CCCC)CCCN
Mol. weight [g/mol]:	186.34
CAS:	102-83-0

Physical Properties

Property code	Value	Unit	Source
gf	218.97	kJ/mol	Joback Method
hf	-169.05	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	52.76	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.237		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
tb	478.20	K	NIST Webbook
tc	707.42	K	Joback Method
tf	329.46	K	Joback Method
vc	0.699	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.47	J/mol×K	536.05	Joback Method
cpg	483.13	J/mol×K	564.61	Joback Method
cpg	499.06	J/mol×K	593.17	Joback Method
cpg	514.29	J/mol×K	621.73	Joback Method
cpg	528.84	J/mol×K	650.29	Joback Method
cpg	542.73	J/mol×K	678.86	Joback Method
cpg	555.98	J/mol×K	707.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102830&Units=SI

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
mccvol:	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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