

N,N'-Bis(diethylaminoethyl)aniline

Other names:	1,1,7,7-Tetraethyl-4-phenyl diethylene triamine N,N-Bis(2-diethylaminoethyl)aniline 1,2-Ethanediamine, N-[2-(diethylamino)ethyl]-N',N'-diethyl-N-phenyl- Diethylenetriamine, 1,1,7,7-tetraethyl-4-phenyl- N-[2-(diethylamino)ethyl]-N',N'-diethyl-N-phenylethylenediamine
Inchi:	InChI=1S/C18H33N3/c1-5-19(6-2)14-16-21(17-15-20(7-3)8-4)18-12-10-9-11-13-18/h9-13
InchiKey:	FPVVUDMZUOYOEU-UHFFFAOYSA-N
Formula:	C18H33N3
SMILES:	CCN(CC)CCN(CCN(CC)CC)c1ccccc1
Mol. weight [g/mol]:	291.47
CAS:	5427-46-3

Physical Properties

Property code	Value	Unit	Source
gf	545.43	kJ/mol	Joback Method
hf	24.27	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	64.07	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	3.177		Crippen Method
mcvol	270.660	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
tb	675.24	K	Joback Method
tc	856.60	K	Joback Method
tf	416.45	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.57	J/molxK	675.24	Joback Method
cpg	796.68	J/molxK	705.47	Joback Method
cpg	815.69	J/molxK	735.69	Joback Method
cpg	833.65	J/molxK	765.92	Joback Method

cpg	850.62	J/mol×K	796.15	Joback Method
cpg	866.66	J/mol×K	826.37	Joback Method
cpg	881.82	J/mol×K	856.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5427463&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
hvp:	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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