

N,N-Bis(2-diethylaminoethyl)aniline

Other names:	1,1,7,7-Tetraethyl-4-phenyl diethylene triamine 1,2-Ethanediamine, N-[2-(diethylamino)ethyl]-N',N'-diethyl-N-phenyl- Diethylenetriamine, 1,1,7,7-tetraethyl-4-phenyl- N,N-Bis(2-diethylaminoethyl)aniline 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]:	291.48

Physical Properties

Property code	Value	Unit	Source
hf	-33.04	kJ/mol	Cheméo Relay (1.0)
hfus	45.48	kJ/mol	Joback Method
hvap	84.81	kJ/mol	Cheméo Relay (1.0)
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-2.48		Cheméo Relay (1.0)
logp	3.177		Crippen Method
mcvol	270.660	ml/mol	McGowan Method
tb	614.03	K	Cheméo Relay (1.0)
tf	247.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5427463&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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