

Demelverine

Other names:	Benzeneethanamine, N-methyl-N-(2-phenylethyl)- Diphenethylamine, N-methyl- Methphenethamine N-Methyl-«beta», «beta»'-diphenyldiethylamine N-Methylbis(2-phenylethyl)amine N-Methyldiphenethylamine
Inchi:	InChI=1S/C17H21N/c1-18(14-12-16-8-4-2-5-9-16)15-13-17-10-6-3-7-11-17/h2-11H,12-15
InchiKey:	XVWQQNARVMHZBP-UHFFFAOYSA-N
Formula:	C17H21N
SMILES:	CN(CCc1ccccc1)CCc1ccccc1
Mol. weight [g/mol]:	239.36
CAS:	13977-33-8

Physical Properties

Property code	Value	Unit	Source
gf	427.86	kJ/mol	Joback Method
hf	146.38	kJ/mol	Joback Method
hfus	30.89	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.404		Crippen Method
mcvol	212.850	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	654.16	K	Joback Method
tc	876.39	K	Joback Method
tf	366.66	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.52	J/molxK	654.16	Joback Method
cpg	582.66	J/molxK	691.20	Joback Method
cpg	600.44	J/molxK	728.24	Joback Method

cpg	616.95	J/mol×K	765.28	Joback Method
cpg	632.26	J/mol×K	802.32	Joback Method
cpg	646.46	J/mol×K	839.36	Joback Method
cpg	659.65	J/mol×K	876.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.70	K	2.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13977338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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