

Nortriptyline

Other names:

Pamelor
1-Propanamine,
3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N-methyl-
5H-Dibenzo[a,d]cycloheptene-«DELTA»5, «gamma»-propylamine,
10,11-dihydro-N-methyl-
Ateben
Avantyl
Aventyl
Demethylamitriptyline
Desitriptilina
Desmethylamitriptyline
Lumbeck
Noramitriptyline
Noritren
5-[3-(Methylamino)propylidene]dibenzo[a,e]cyclohepta[1,5]diene
Amitriptyline, demethyl-
Demethylamitriptylene
Demethylamitriptyline
10,11-Dihydro-N-methyl-5H-dibenzo(a,d)cycloheptane-«DELTA», «gamma»-propylamine
5-(3-Methylaminopropylidene)-10,11-dihydro-5H-dibenzo(a,d)cycloheptene
3-(10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N-methylpropylamine
Sesaval
10,11-Dihydro-5-(3-methylaminopropylidene)-5H-dibenzo[a,d][1,4]cycloheptene
Nortryptiline
Nortriptylene

Inchi: InChI=1S/C19H21N/c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16-8-3-5-10-18(16)19/h2-
InchiKey: PHVGLTMQBUIQQ-UHFFFAOYSA-N
Formula: C19H21N
SMILES: CNCCC=C1c2cccc2CCc2cccc21
Mol. weight [g/mol]: 263.38
CAS: 72-69-5

Physical Properties

Property code	Value	Unit	Source
gf	517.97	kJ/mol	Joback Method
hf	237.27	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method

ie	8.39 ± 0.11	eV	NIST Webbook
log10ws	-5.12		Crippen Method
logp	3.826		Crippen Method
mcvol	225.870	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2273.80		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2225.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2202.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2176.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2273.80		NIST Webbook
rinpol	2217.00		NIST Webbook

rinpol	2215.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2214.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2202.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2202.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2215.00		NIST Webbook
ripol	3062.00		NIST Webbook
ripol	3062.00		NIST Webbook
tb	765.66	K	Joback Method
tc	1002.96	K	Joback Method
tf	466.97	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.75	J/molxK	765.66	Joback Method
cpg	662.82	J/molxK	805.21	Joback Method
cpg	678.73	J/molxK	844.76	Joback Method
cpg	693.61	J/molxK	884.31	Joback Method
cpg	707.58	J/molxK	923.86	Joback Method
cpg	720.78	J/molxK	963.41	Joback Method
cpg	733.33	J/molxK	1002.96	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=C72695&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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