Benadryl

Other names:

2-(Benzhydryloxy)-N,N-Dimethylethylamine
2-(Benzohydryloxy)-N,N-dimethylethylamine
2-(Diphenylmethoxy)-N,N-dimethylethylamine
Aleryl
Alledryl
Allergan B
Allergeval
Allergical
Allergina
Allergival
Amidryl
Antistominum
Antomin
Bagodryl
Baramine
Ben-allergin
Bena
Benachlor
Benadrin
Benapon
Benodin
Benodine
Benylan
Benzantine
Benzhydramine
Benzhydraminum
Benzhydril
Benzhydroamina
Benzhydryl
Betramin
Dabylen
Debendrin
Dermistina
Dermodrin
Desentol
Diabenyl
Diabylen
Dibendrin
Dibondrin
Difedryl

Difenhydramin
Difenidramina
Dihidral
Dimedrol
Dimedrol base
Dimedryl
Diphantine
Diphenhydramine
Diphenylhydramine
Diphenylmethanol, (N,N-dimenthylaminoethyl) ether
Dryistan
Drylistan
Dylamon
Etanautine
Ethanamine, 2-(diphenylmethoxy)-N,N-dimethyl-
Ethylamine, 2-(diphenylmethoxy)-N,N-dimethyl-
Ethylamine, N,N-dimethyl-2-(diphenylmethoxy)-
FAR 90X2
Histaxin
Hyadrine
Ibiodral
Medidryl
Mephadryl
N,N-Dimethyl-2-diphenylmethyloxyethylamine
N-(Benzhydryloksy-etylo)dwumetyloamina
N-[2-(Diphenylmethoxy)ethyl]-N,N-dimethylamine
Nausen
Novamina
O-Benzhydryl(dimethylamino)ethanol
PM 255
Probedryl
Rigidil
Rigidyl
S 51
Syntedril
Syntodril
deprenyl
«alpha»-(2-Dimethylaminoethoxy)diphenylmethane
«beta»-(Dimethylamino)ethanol diphenylmethyl ether
«beta»-(Dimethylamino)ethyl benzhydryl ether
«beta»-Dimethylamino-aethyl-benzhydryl-aether
Â«alphaÂ»-(2-Dimethylaminoethoxy)diphenylmethane
Â«betaÂ»-(Dimethylamino)ethanol diphenylmethyl ether

	Â«betaÂ»-(Dimethylamino)ethyl benzhydryl ether
	Â«betaÂ»-Dimethylamino-aethyl-benzhydryl-aether
Inchi:	InChI=1S/C17H21NO/c1-18(2)13-14-19-17(15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3-12,1
InchiKey:	ZZVUWRFHKOJYTH-UHFFFAOYSA-N
Formula:	C17H21NO
SMILES:	CN(C)CCOC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	255.35
CAS:	58-73-1

Physical Properties

Property code	Value	Unit	Source
gf	320.42	kJ/mol	Joback Method
hf	8.88	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-2.51		Aqueous Solubility Prediction Method
logp	3.354		Crippen Method
mcvol	218.720	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1841.00		NIST Webbook

rinpol	1865.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1874.00		NIST Webbook
ripol	2513.00		NIST Webbook
tb	676.14	K	Joback Method
tc	899.87	K	Joback Method
tf	373.89	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.33	J/mol×K	676.14	Joback Method
cpg	611.23	J/mol×K	713.43	Joback Method
cpg	628.78	J/mol×K	750.72	Joback Method
cpg	645.04	J/mol×K	788.01	Joback Method
cpg	660.08	J/mol×K	825.30	Joback Method
cpg	673.97	J/mol×K	862.58	Joback Method
cpg	686.79	J/mol×K	899.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58731&Units=SI

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

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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