Amodryl

Other names:	Bromazine
	Bromdiphenhydramine
	Ethanamine, 2-[(4-bromophenyl)phenylmethoxy]-N,N-dimethyl-
	Ethylamine, 2-[(p-bromo-«alpha»-phenylbenzyl)oxy]-N,N-dimethyl-
	«beta»-(p-Bromobenzhydryloxy)ethyldimethylamine
	Ambodryl
	Bromanautine
	Bromazin base
	Bromo-Benadryl
	Bromo-Benadryl base
	Bromodiphenhydramine
	Deserol
	Deserol base
	Histabromamine
	Neo-Benadryl
	2-[(p-Bromo-«alpha»-phenylbenzyl)oxy]-N,N-dimethylethylamine
Inchi:	InChI=1S/C17H20BrNO/c1-19(2)12-13-20-17(14-6-4-3-5-7-14)15-8-10-16(18)11-9-15/h3
InchiKey:	NUNIWXHYABYXKF-UHFFFAOYSA-N
Formula:	C17H20BrNO
SMILES:	CN(C)CCOC(c1ccccc1)c1ccc(Br)cc1
Mol. weight [g/mol]:	334.25
CAS:	118-23-0

Physical Properties

Property code	Value	Unit	Source
gf	325.11	kJ/mol	Joback Method
hf	23.74	kJ/mol	Joback Method
hfus	33.45	kJ/mol	Joback Method
hvap	69.15	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.117		Crippen Method
mcvol	236.220	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook

rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2155.00		NIST Webbook
ripol	2942.00		NIST Webbook
ripol	2942.00		NIST Webbook
tb	747.28	K	Joback Method
tc	982.07	K	Joback Method
tf	446.21	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.19	J/mol×K	747.28	Joback Method
cpg	651.89	J/mol×K	786.41	Joback Method
cpg	667.29	J/mol×K	825.54	Joback Method
cpg	681.48	J/mol×K	864.68	Joback Method
cpg	694.55	J/mol×K	903.81	Joback Method
cpg	706.58	J/mol×K	942.94	Joback Method
cpg	717.65	J/mol×K	982.07	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C118230&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
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