Ethylamine, 2-((p-bromo-«alpha»-methyl-«alpha»-phenylbenzy

Other names: 2-((p-Bromo-«alpha»-methyl-«alpha»-phenylbenzyl)oxy)-N,N-dimethylethylamine
Embramine
Ethanamine, 2-(1-(4-bromophenyl)-1-phenylethoxy)-N,N-dimethyl-
Mebrophenhydramine

Inchi: InChI=1S/C18H22BrNO/c1-18(21-14-13-20(2)3,15-7-5-4-6-8-15)16-9-11-17(19)12-10-16

InchiKey: URSRSKSNFPUKGH-UHFFFAOYSA-N

Formula: C18H22BrNO

SMILES: CN(C)CCOC(C)(c1ccccc1)c1ccc(Br)cc1

Mol. weight [g/mol]: 348.28

CAS: 3565-72-8

Physical Properties

Property code	Value	Unit	Source
gf	338.81	kJ/mol	Joback Method
hf	-0.37	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	70.47	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.291		Crippen Method
mcvol	250.310	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	767.37	K	Joback Method
tc	1005.75	K	Joback Method
tf	474.90	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.93	J/mol×K	767.37	Joback Method
cpg	709.00	J/mol×K	807.10	Joback Method
cpg	724.73	J/mol×K	846.83	Joback Method

cpg	739.23	J/mol×K	886.56	Joback Method
cpg	752.62	J/mol×K	926.29	Joback Method
cpg	765.03	J/mol×K	966.02	Joback Method
cpg	776.56	J/mol×K	1005.75	Joback Method

Sources

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=C3565728&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume