Phenacaine

Other names:	Acetamidine, N,N'-bis(p-ethoxyphenyl)- N,N'-Bis(p-ethoxyphenyl)acetamidine N',N
Inchi:	InChI=1S/C18H22N2O2/c1-4-21-17-10-6-15(7-11-17)19-14(3)20-16-8-12-18(13-9-16)22-
InchiKey:	QXDAEKSDNVPFJG-UHFFFAOYSA-N
Formula:	C18H22N2O2
SMILES:	CCOc1ccc(N=C(C)Nc2ccc(OCC)cc2)cc1
Mol. weight [g/mol]:	298.38
CAS:	101-93-9

Physical Properties

Property code	Value	Unit	Source
hf	-103.27	kJ/mol	Joback Method
hvap	76.19	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.646		Crippen Method
mcvol	244.360	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	846.13	K	Joback Method
tc	1078.34	K	Joback Method

Sources

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=C101939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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