

Morpholine, 4-[3-(4-butoxyphenoxy)propyl]-

Other names:

Morpholine, 4-(3-(p-butoxyphenoxy)propyl)-
4-(3-(p-Butoxyphenoxy)propyl)morpholine
p-Butoxyphenyl «gamma»-morpholinopropyl ether
«gamma»-Morpholinopropyl 4-n-butoxyphenyl ether
Pramocaine
Pramoxine
Tronopthane
Tronothane
Proxazocain

Inchi:

InChI=1S/C17H27NO3/c1-2-3-12-20-16-5-7-17(8-6-16)21-13-4-9-18-10-14-19-15-11-18/

InchiKey:

DQKXQSGTHWVTAD-UHFFFAOYSA-N

Formula:

C17H27NO3

SMILES:

CCCCOc1ccc(OCCCN2CCOCC2)cc1

Mol. weight [g/mol]:

293.40

CAS:

140-65-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.967		Crippen Method
mcvol	243.360	ml/mol	McGowan Method
rinpol	2263.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2281.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C140658&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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