

Buclizine

Other names:

Piperazine,
1-[[4-(4-chlorophenyl)phenylmethyl]-4-[[4-(1,1-dimethylethyl)phenyl]methyl]-
Piperazine, 1-(p-tert-butylbenzyl)-4-(p-chloro-«alpha»-phenylbenzyl)-

Aphilan-R base

AH 2526

Buclifen

Histabuticine

Histabutizine

Histabutyazine

Vibazine

1-(p-tert-Butylbenzyl)-4-(p-chloro-«alpha»-phenylbenzyl)piperazine

Hitabutyzyne

Posdel

Postafen

Inchi:

InChI=1S/C28H33ClN2/c1-28(2,3)25-13-9-22(10-14-25)21-30-17-19-31(20-18-30)27(23-

InchiKey:

MOYGZHXDRJNJEP-UHFFFAOYSA-N

Formula:

C28H33ClN2

SMILES:

CC(C)(C)c1ccc(CN2CCN(C(c3ccccc3)c3ccc(Cl)cc3)CC2)cc1

Mol. weight [g/mol]:

433.03

CAS:

82-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.27		Crippen Method
logp	6.545		Crippen Method
mcpvol	355.440	ml/mol	McGowan Method
rinpol	3267.00		NIST Webbook
rinpol	3285.00		NIST Webbook
rinpol	3295.00		NIST Webbook
rinpol	3290.00		NIST Webbook
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
rinpol	3286.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C82951&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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