Terfenadine

Other names:

(.+/-.)-Terfenadine
1-Piperidinebutanol, «alpha»-[4-(1,1-dimethylethyl)phenyl]-4-(hydroxydiphenylmethyl)-
1-Piperidinebutanol, Â«alphaÂ»-[4-(1,1-dimethylethyl)phenyl]-4-(hydroxydiphenylmethyl)-
Aldaban
Allerplus
Cyater
MDL-9918
Nebralin
RMI 9918
Seldane
Teldane
Teldanex
Terdin
Terfex
Ternadin
Triludan
«alpha»-(4-(1,1-Dimethylethyl)phenyl)-4-(hydroxydiphenylmethyl)-1-piperidinebutanol
«alpha»-(p-tert-Butylphenyl)-4-(hydroxydiphenylmethyl)-1-piperidinebutanol
«alpha»-[4-(1,1-dimethylethyl)phenyl]-4-(hydroxydiphenylmethyl)-1-piperidinebutanol (terfenadine)
Â«alphaÂ»-(4-(1,1-Dimethylethyl)phenyl)-4-(hydroxydiphenylmethyl)-1-piperidinebutanol
Â«alphaÂ»-(p-tert-Butylphenyl)-4-(hydroxydiphenylmethyl)-1-piperidinebutanol
Â«alphaÂ»-[4-(1,1-dimethylethyl)phenyl]-4-(hydroxydiphenylmethyl)-1-piperidinebutanol (terfenadine)

Inchi: InChI=1S/C32H41NO2/c1-31(2,3)26-18-16-25(17-19-26)30(34)15-10-22-33-23-20-29(21

InchiKey: GUGOEEXESWIERI-UHFFFAOYSA-N

Formula: C32H41NO2

SMILES: CC(C)(C)c1ccc(C(O)CCCN2CCC(C(O)(c3ccccc3)c3ccccc3)CC2)cc1

Mol. weight [g/mol]: 471.67

CAS: 50679-08-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Aqueous Solubility Prediction Method
log10ws	-7.74		Aqueous Solubility Prediction Method
logp	6.446		Crippen Method
mcvol	401.320	ml/mol	McGowan Method

tf	420.40	K	Aqueous Solubility Prediction Method
tf	420.40	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	58.10	kJ/mol	422.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50679088&Units=SI

Legend

hfust: Enthalpy of fusion at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point