

2,2-Dimethyl-1-(2'-methyl-delta²-pentenyl)-3-piperazine

Other names:	2,2-Dimethyl-1-(2'-methyl-delta
Inchi:	InChI=1S/C12H22N2O/c1-5-6-10(2)9-14-8-7-13-11(15)12(14,3)4/h6H,5,7-9H2,1-4H3,(H,
InchiKey:	UVAPKZXGLILQIU-UXBLZVDNSA-N
Formula:	C12H22N2O
SMILES:	CCC=C(C)CN1CCN=C(O)C1(C)C
Mol. weight [g/mol]:	210.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	2.393		Crippen Method
mcvol	186.310	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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