

Dexetimide

Other names:	[3,4'-Bipiperidine]-2,6-dione, 3-phenyl-1'-(phenylmethyl)-, (S)-(+)-2-(1-Benzyl-4-piperidyl)-2-phenylglutarimide Dexbenzetimide Dextrobenzetimide
Inchi:	InChI=1S/C23H26N2O2/c26-21-11-14-23(22(27)24-21,19-9-5-2-6-10-19)20-12-15-25(16
InchiKey:	LQQIVYSCPWCSSD-UHFFFAOYSA-N
Formula:	C23H26N2O2
SMILES:	O=C1CCC(c2ccccc2)(C2CCN(Cc3ccccc3)CC2)C(=O)N1
Mol. weight [g/mol]:	362.46
CAS:	21888-98-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	3.273		Crippen Method
mcvol	288.790	ml/mol	McGowan Method
rinpol	3127.00		NIST Webbook
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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=C21888982&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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