

Norpipanone

Other names:	3-Hexanone, 4,4-diphenyl-6-(1-piperidiny)- 3-Hexanone, 4,4-diphenyl-6-piperidino- Hexalgon Hoechst 10,495 Hoechst 10495 Orfenso 4,4-Diphenyl-6-(1-piperidyl)-3-hexanone 1-Piperidino-3,3-diphenyl-4-hexanone
Inchi:	InChI=1S/C23H29NO/c1-2-22(25)23(20-12-6-3-7-13-20,21-14-8-4-9-15-21)16-19-24-17-
InchiKey:	WCDSHELZWCOTMI-UHFFFAOYSA-N
Formula:	C23H29NO
SMILES:	CCC(=O)C(CCN1CCCCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	335.48
CAS:	561-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.828		Crippen Method
mcvol	288.100	ml/mol	McGowan Method
rinsol	2488.00		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=C561488&Units=SI

Legend

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

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