

Dipipanone

Other names:	3-Heptanone, 4,4-diphenyl-6-(1-piperidiny)- 3-Heptanone, 4,4-diphenyl-6-piperidino- Dipipanon Piperidyl amidone 4,4-Diphenyl-6-piperidino-3-heptanone Fenpidon Pamedon(e) Pipadone
Inchi:	InChI=1S/C24H31NO/c1-3-23(26)24(21-13-7-4-8-14-21,22-15-9-5-10-16-22)19-20(2)25-
InchiKey:	SVDHSZFEQYXRDC-UHFFFAOYSA-N
Formula:	C24H31NO
SMILES:	CCC(=O)C(CC(C)N1CCCCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	349.51
CAS:	467-83-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	5.216		Crippen Method
mcvol	302.190	ml/mol	McGowan Method
rinpol	2474.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2467.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C467834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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