

Phenoperidine

Other names:	4-Piperidinecarboxylic acid, 1-(3-hydroxy-3-phenylpropyl)-4-phenyl-, ethyl ester 1-(3-Hydroxy-3-phenylpropyl)-4-phenylpiperidine-4-carboxylic acid ethyl ester Phenoperidin R-1406
Inchi:	InChI=1S/C23H29NO3/c1-2-27-22(26)23(20-11-7-4-8-12-20)14-17-24(18-15-23)16-13-2
InchiKey:	IPOPQVVNCFQFRK-UHFFFAOYSA-N
Formula:	C23H29NO3
SMILES:	CCOC(=O)C1(c2ccccc2)CCN(CCC(O)c2ccccc2)CC1
Mol. weight [g/mol]:	367.48
CAS:	562-26-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	3.707		Crippen Method
mcvol	299.840	ml/mol	McGowan Method
rinsol	2872.00		NIST Webbook
rinsol	2872.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C562265&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

Latest version available from:

<https://www.chemeo.com/cid/99-092-1/Phenoperidine.pdf>

Generated by Cheméo on 2024-04-23 21:32:32.375615318 +0000 UTC m=+16197201.296192634.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.