Piperine

Other names:	1,3-Benzodioxol-5-yl-1-oxo-2,4-pentadienyl-piperidine
	1-Piperoylpiperidine
	5-(Methylenedioxyphenyl)-2,4-pentadienoyl piperidide (Piperin)
	Piperidine, 1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]-, (E,E)-
	Piperidine, 1-piperoyl-, (E,E)-
	Piperin
Inchi:	InChI=1S/C17H19NO3/c19-17(18-10-4-1-5-11-18)7-3-2-6-14-8-9-15-16(12-14)21-13-20-
InchiKey:	MXXWOMGUGJBKIW-YPCIICBESA-N
Formula:	C17H19NO3
SMILES:	O=C(C=CC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]:	285.34
CAS:	94-62-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Aqueous Solubility Prediction Method
log10ws	-3.46		Estimated Solubility Method
logp	2.997		Crippen Method
mcvol	219.600	ml/mol	McGowan Method
rinpol	2933.00		NIST Webbook
rinpol	2835.00		NIST Webbook
rinpol	2835.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tf	404.40	K	Aqueous Solubility Prediction Method
tf	388.00 ± 2.00	K	NIST Webbook
tf	399.00 ± 2.00	K	NIST Webbook
tf	403.00 ± 2.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94622&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point