Papaverine

Other names:	1-((3,4-Dimethoxyphenyl)methyl)-6,7-dimethoxyisoquinoline 1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxyisoquinoline 6,7-Dimethoxy-1-veratrylisoquinoline Isoquinoline, 1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy- Isoquinoline, 6,7-dimethoxy-1-veratryl- NSC 136630 Papanerine Papaverin Papaverina Robaxapap S-M-R
Inchi:	InChI=1S/C20H21NO4/c1-22-17-6-5-13(10-18(17)23-2)9-16-15-12-20(25-4)19(24-3)11-1
InchiKey:	XQYZDYMELSJDRZ-UHFFFAOYSA-N
Formula:	C20H21NO4
SMILES:	COc1ccc(Cc2nccc3cc(OC)c(OC)cc23)cc1OC
Mol. weight [g/mol]:	339.38
CAS:	58-74-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Aqueous Solubility Prediction Method
logp	3.860		Crippen Method
mcvol	259.140	ml/mol	McGowan Method
rinpol	2814.00		NIST Webbook
rinpol	2818.00		NIST Webbook
rinpol	2808.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2840.00		NIST Webbook
rinpol	2806.00		NIST Webbook
rinpol	2824.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2819.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2825.00		NIST Webbook

rinpol	2780.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2770.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2815.00		NIST Webbook
tf	420.40	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58742&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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