Ancymidol

Other names:	5-Pyrimidinemethanol, «alpha»-cyclopropyl-«alpha»-(4-methoxyphenyl)- 5-Pyrimidinemethanol, «alpha»-cyclopropyl-«alpha»-(p-methoxyphenyl)- 5-Pyrimidinemethanol, Â«alphaÂ»-cyclopropyl-Â«alphaÂ»-(4-methoxyphenyl)- 5-Pyrimidinemethanol, Â«alphaÂ»-cyclopropyl-Â«alphaÂ»-(p-methoxyphenyl)- «alpha»-cyclopropyl-«alpha»-(4-methoxyphenyl)-5-pyrimidinemethanol «alpha»-cyclopropyl-«alpha»-(4-methoxyphenyl)-5-pyrimidylmethanol Â«alphaÂ»-cyclopropyl-Â«alphaÂ»-(4-methoxyphenyl)-5-pyrimidinemethanol Â«alphaÂ»-cyclopropyl-Â«alphaÂ»-(4-methoxyphenyl)-5-pyrimidylmethanol
Inchi:	InChI=1S/C15H16N2O2/c1-19-14-6-4-12(5-7-14)15(18,11-2-3-11)13-8-16-10-17-9-13/h4
InchiKey:	HUTDUHSNJYTCAR-UHFFFAOYSA-N
Formula:	C15H16N2O2
SMILES:	COc1ccc(C(O)(c2cncnc2)C2CC2)cc1
Mol. weight [g/mol]:	256.30
CAS:	12771-68-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Aqueous Solubility Prediction Method
log10ws	-2.60		Estimated Solubility Method
logp	2.131		Crippen Method
mcvol	195.530	ml/mol	McGowan Method
rinpol	2187.00		NIST Webbook
rinpol	2244.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tf	383.65	K	Aqueous Solubility Prediction Method
tf	384.57 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.63	kJ/mol	383.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C12771685&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
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