Ketobemidone

Other names: 1-Propanone, 1-[4-(3-hydroxyphenyl)-1-methyl-4-piperidinyl]-
1-Propanone, 1-[4-(m-hydroxyphenyl)-1-methyl-4-piperidyl]-
A 21 Lundbeck
Cetobemidon
Cetobemidone
Ciba 7115
Cliradon
Cliradone
Cymidon
Hoechst 10720
K 4710
Win 1539
Ethyl (4-(m-hydroxyphenyl)-1-methyl)-4-piperidyl ketone
Ketone, ethyl 4-(m-hydroxyphenyl)-1-methylpiperidyl
1-(4-(m-Hydroxyphenyl)-1-methyl-4-piperidyl)-1-propanone
4-(m-Hydroxyphenyl)-1-methyl-4-propionylpiperidine
4-(m-Hydroxyphenyl)-1-methyl-4-piperidyl ethyl ketone
NSC 117863

Inchi: InChI=1S/C15H21NO2/c1-3-14(18)15(7-9-16(2)10-8-15)12-5-4-6-13(17)11-12/h4-6,11,17

InchiKey: ALFGKMXHOUSVAD-UHFFFAOYSA-N

Formula: C15H21NO2

SMILES: CCC(=O)C1(c2cccc(O)c2)CCN(C)CC1

Mol. weight [g/mol]: 247.33

CAS: 469-79-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	2.335		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	2060.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2035.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C469794&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices