

Fenyramidol

Other names:

Benzenemethanol, «alpha»-[(2-pyridinylamino)methyl]-
Benzyl alcohol, «alpha»-[(2-pyridylamino)methyl]-
«alpha»-[(2-Pyridylamino)methyl]benzyl alcohol
Cabral
Evasprin
IN 511
MJ 505
Phenylramidol
Phenyramidol
2-(«beta»-Hydroxyphenethylamino)pyridine
Bonapar
Evaspirine
Evasprine
Vilexin
Pyridine, 2-(«beta»-hydroxyphenethylamino)-
(./-.)-Phenyramidol
NSC 23634
Pyridine, 2-(beta-hydroxyphenethylamino)-

Inchi:

InChI=1S/C13H14N2O/c16-12(11-6-2-1-3-7-11)10-15-13-8-4-5-9-14-13/h1-9,12,16H,10H

InchiKey:

ZEAJXCPGHPJVNP-UHFFFAOYSA-N

Formula:

C13H14N2O

SMILES:

OC(CNc1ccccn1)c1cccc1

Mol. weight [g/mol]:

214.26

CAS:

553-69-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	2.227		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
rinpol	1957.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	2006.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C553695&Units=SI

Legend

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

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