

Nefopam

Other names:	1H-2,5-Benzoxazocine, 3,4,5,6-tetrahydro-5-methyl-1-phenyl-Fenazoxine 3,4,5,6-Tetrahydro-5-methyl-2-phenyl-1H-2,5-benzoxazocine
Inchi:	InChI=1S/C17H19NO/c1-18-11-12-19-17(14-7-3-2-4-8-14)16-10-6-5-9-15(16)13-18/h2-1
InchiKey:	RGPDEAGGEXEMMM-UHFFFAOYSA-N
Formula:	C17H19NO
SMILES:	CN1CCOC(c2ccccc2)c2ccccc2C1
Mol. weight [g/mol]:	253.34
CAS:	13669-70-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	3.238		Crippen Method
mcvol	207.860	ml/mol	McGowan Method
rinsol	2017.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13669700&Units=SI
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

Legend

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

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