

1-(Beta-cyanoethyl)-4-phenyl-4-piperidinol

Inchi:	InChI=1S/C14H18N2O/c15-9-4-10-16-11-7-14(17,8-12-16)13-5-2-1-3-6-13/h1-3,5-6,17H,
InchiKey:	YFHOEXZVEVBIHH-UHFFFAOYSA-N
Formula:	C14H18N2O
SMILES:	N#CCCN1CCC(O)(c2ccccc2)CC1
Mol. weight [g/mol]:	230.31
CAS:	5193-57-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.884		Crippen Method
mcvol	190.730	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5193577&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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