

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,1-2,14,15,16,18H,19H,20H
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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5193577&Units=SI>
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>

Legend

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

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<https://www.chemeo.com/cid/55-006-4/1-Beta-cyanoethyl-4-phenyl-4-piperidinol.pdf>

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