

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

Inchi: InChI=1S/C16H23NO3/c1-2-20-15(18)8-11-17-12-9-16(19,10-13-17)14-6-4-3-5-7-14/h3-7
InchiKey: ZOSSQUOBDBJSIE-UHFFFAOYSA-N
Formula: C16H23NO3
SMILES: CCOC(=O)CCN1CCC(O)(c2ccccc2)CC1
Mol. weight [g/mol]: 277.36
CAS: 116660-52-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	1.923		Crippen Method
mcvol	224.970	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=C116660527&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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