Phenol, 3,5-bis(1-pyrrolidinyl)-

Other names: 3,5-Di-pyrrolidin-1-yl-phenol
Inchi: InChI=1S/C14H20N2O/c17-14-10-12(15-5-1-2-6-15)9-13(11-14)16-7-3-4-8-16/h9-11,17H
InchiKey: LABWUCJZQBDUAV-UHFFFAOYSA-N
Formula: C14H20N2O
SMILES: Oc1cc(N2CCCC2)cc(N2CCCC2)c1
Mol. weight [g/mol]: 232.32
CAS: 16857-92-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.593		Crippen Method
mcvol	188.470	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16857924&Units=SI

Legend

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