4-(2-(Pyridin-2-yl)ethyl)phenol

Inchi: InChI=1S/C13H13NO/c15-13-8-5-11(6-9-13)4-7-12-3-1-2-10-14-12/h1-3,5-6,8-10,15H,4,
InchiKey: RZKWYCPJVXNMMC-UHFFFAOYSA-N
Formula: C13H13NO
SMILES: Oc1ccc(CCc2ccccn2)cc1
Mol. weight [g/mol]: 199.25
CAS: 3767-85-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.572		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
rinpol	1900.90		NIST Webbook
rinpol	1900.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3767859&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
rinpol: Non-polar retention indices