

Phenol, 4-methyl-2-(1-piperidinylmethyl)-

Other names:	4-Methyl-2-(1-piperidinylmethyl)phenol 4-Methyl-2-(piperidinomethyl)phenol «alpha»2-piperidino-2,4-xlenol
Inchi:	InChI=1S/C13H19NO/c1-11-5-6-13(15)12(9-11)10-14-7-3-2-4-8-14/h5-6,9,15H,2-4,7-8,1
InchiKey:	SMZFAZCVXCKGAC-UHFFFAOYSA-N
Formula:	C13H19NO
SMILES:	Cc1ccc(O)c(CN2CCCCC2)c1
Mol. weight [g/mol]:	205.30
CAS:	21236-74-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	2.687		Crippen Method
mcvol	175.260	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	0.03	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21236748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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