

Piperidine, 1-(phenylmethyl)-

Other names:	1-benzylpiperidine
Inchi:	InChI=1S/C12H17N/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h1,3-4,7-8H,2,5-6,9-11H2
InchiKey:	NZVZVGPYTICZBZ-UHFFFAOYSA-N
Formula:	C12H17N
SMILES:	c1ccc(CN2CCCCC2)cc1
Mol. weight [g/mol]:	175.27
CAS:	2905-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.673		Crippen Method
mccvol	155.300	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.70	K	2.80	NIST Webbook
tbrp	406.50 ± 0.50	K	2.80	NIST Webbook

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=C2905568&Units=SI

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

Latest version available from:

<https://www.cheméo.com/cid/75-445-5/Piperidine-1-phenylmethyl.pdf>

Generated by Cheméo on 2024-04-26 04:28:48.391642628 +0000 UTC m=+16394977.312219951.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.