

4-Piperidinone, 1-(phenylmethyl)-

Other names:	1-Benzyl-4-oxopiperidine N-Benzylpiperidinone N-Benzyl-4-piperidinone 1-Benzyl-4-piperidinone N-Benzyl-4-piperidone 1-Benzylpiperidone 1-Benzyl-4-piperidone 4-Piperidone, 1-benzyl- N-Benzylpiperidin-4-one 4-N-Benzylpiperidone
Inchi:	InChI=1S/C12H15NO/c14-12-6-8-13(9-7-12)10-11-4-2-1-3-5-11/h1-5H,6-10H2
InchiKey:	SJZKULRDWHPHGG-UHFFFAOYSA-N
Formula:	C12H15NO
SMILES:	O=C1CCN(Cc2ccccc2)CC1
Mol. weight [g/mol]:	189.25
CAS:	3612-20-2

Physical Properties

Property code	Value	Unit	Source
hvap	78.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.19		Crippen Method
logp	1.852		Crippen Method
mcvol	156.870	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.20	K	0.90	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=C3612202&Units=SI>

Legend

h_{vap}: Enthalpy of vaporization at standard conditions
log₁₀ws: Log₁₀ of Water solubility in mol/l
log_p: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
t_{brp}: Boiling point at reduced pressure

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