

4-Piperidinone, 1-benzoyl-

Other names:	1-Benzoyl-4-oxopiperidine 1-Benzoyl-4-piperidinone N-Benzoyl-4-piperidone 1-Benzoyl-4-piperidone 4-Piperidone, 1-benzoyl- 1-Benzoyl-piperidinoine 1-Benzoyl-piperidin-4-one
Inchi:	InChI=1S/C12H13NO2/c14-11-6-8-13(9-7-11)12(15)10-4-2-1-3-5-10/h1-5H,6-9H2
InchiKey:	NZAXGZYPZGEVBD-UHFFFAOYSA-N
Formula:	C12H13NO2
SMILES:	O=C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]:	203.24
CAS:	24686-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	1.492		Crippen Method
mcvol	158.440	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.20	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=C24686780&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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