

Indole, 3-benzoyl-

Other names:	Methanone, 1H-indol-3-ylphenyl- 3-Benzoylindole Ketone, indol-3-yl phenyl
Inchi:	InChI=1S/C15H11NO/c17-15(11-6-2-1-3-7-11)13-10-16-14-9-5-4-8-12(13)14/h1-10,16H
InchiKey:	ADHQLIGSIQGNBW-UHFFFAOYSA-N
Formula:	C15H11NO
SMILES:	O=C(c1cccc1)c1c[nH]c2cccc12
Mol. weight [g/mol]:	221.25
CAS:	15224-25-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	2.917		Crippen Method
mcvol	171.080	ml/mol	McGowan Method

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=C15224256&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/84-992-8/Indole-3-benzoyl.pdf>

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