Phenyl 4-pyridyl ketone

Other names:	Methanone, phenyl-4-pyridinyl- Ketone, phenyl 4-pyridyl «gamma»-Benzoylpyridine Ba 33215 4-Benzoylpyridine 4-Pyridyl phenyl ketone Pyridine, 4-benzoyl- Phenyl(4-pyridinyl)methanone NSC 9488
Inchi:	InChI=1S/C12H9NO/c14-12(10-4-2-1-3-5-10)11-6-8-13-9-7-11/h1-9H
InchiKey:	SKFLCXNDKRUHTA-UHFFFAOYSA-N
Formula:	C12H9NO
SMILES:	O=C(c1ccccc1)c1ccncc1
Mol. weight [g/mol]:	183.21
CAS:	14548-46-0

Physical Properties

Property code	Value	Unit	Source
ie	9.60 ± 0.10	eV	NIST Webbook
log10ws	-3.20		Crippen Method
logp	2.313		Crippen Method
mcvol	143.970	ml/mol	McGowan Method
tb	588.20	K	NIST Webbook
tb	588.00	K	NIST Webbook
tf	348.00 ± 1.50	K	NIST Webbook
tf	345.10 ± 0.50	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14548460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point