Phenyl 3-pyridyl ketone

Other names:	Methanone, phenyl-3-pyridinyl-
	Ketone, phenyl 3-pyridyl
	3-Benzoylpyridine
	Pyridine, 3-benzoyl-
	3-Pyridyl phenyl ketone
Inchi:	InChI=1S/C12H9NO/c14-12(10-5-2-1-3-6-10)11-7-4-8-13-9-11/h1-9H
InchiKey:	RYMBAPVTUHZCNF-UHFFFAOYSA-N
Formula:	C12H9NO
SMILES:	O=C(c1ccccc1)c1cccnc1
Mol. weight [g/mol]:	183.21
CAS:	5424-19-1

Physical Properties

Property code	Value	Unit	Source
affp	934.10	kJ/mol	NIST Webbook
basg	902.30	kJ/mol	NIST Webbook
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	580.20	K	NIST Webbook
tb	591.70	K	NIST Webbook
tb	591.50 ± 0.50	K	NIST Webbook
tf	315.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.00 ± 1.00	K	0.34	NIST Webbook

Sources

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=C5424191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point