Methanone, phenyl-2-pyridinyl-

Other names:	Ketone, phenyl 2-pyridyl
	Phenyl 2-pyridyl ketone
	2-Benzoylpyridine
	Pyridine, 2-benzoyl-
Inchi:	InChI=1S/C12H9NO/c14-12(10-6-2-1-3-7-10)11-8-4-5-9-13-11/h1-9H
InchiKey:	GCSHUYKULREZSJ-UHFFFAOYSA-N
Formula:	C12H9NO
SMILES:	O=C(c1ccccc1)c1ccccn1
Mol. weight [g/mol]:	183.21
CAS:	91-02-1

Physical Properties

Property code	Value	Unit	Source
ie	9.06	eV	NIST Webbook
ie	9.06	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-3.20		Crippen Method
logp	2.313		Crippen Method
mcvol	143.970	ml/mol	McGowan Method
tb	590.20	K	NIST Webbook
tb	590.00	K	NIST Webbook
tf	316.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.91	kJ/mol	210.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	444.20	K	1.30	NIST Webbook
tbrp	444.00 ± 1.00	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91021&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

hfust:	Enthalpy of fusion at a given temperature
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