METHANONE, DI-2-PYRIDINYL-

Other names:	2,2'-Dipyridyl ketone
	Methanone, di-2-pyridinyl-
	2-Pyridyl ketone
	Ketone, di-2-pyridyl
	Bis(2-pyridyl) ketone
	Di(pyridin-2-yl) ketone
	Di(2-pyridinyl)methanone
Inchi:	InChI=1S/C11H8N2O/c14-11(9-5-1-3-7-12-9)10-6-2-4-8-13-10/h1-8H
InchiKey:	QPOWUYJWCJRLEE-UHFFFAOYSA-N
Formula:	C11H8N2O
SMILES:	O=C(c1ccccn1)c1ccccn1
Mol. weight [g/mol]:	184.20

Physical Properties

Property code	Value	Unit	Source
af	0.5158		Cheméo Relay (1.0)
gf	191.39	kJ/mol	Cheméo Relay (1.0, beta)
hf	150.58	kJ/mol	Cheméo Relay (1.0)
hvap	81.89	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-1.88		Cheméo Relay (1.0)
logp	1.708		Crippen Method
mcvol	139.860	ml/mol	McGowan Method
pc	4148.03	kPa	Cheméo Relay (1.0, beta)
tb	595.23	K	Cheméo Relay (1.0)
tc	859.79	K	Cheméo Relay (1.0)
tf	383.61	K	Cheméo Relay (1.0)
vc	0.527	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19437264&Units=SI

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume