2-(2-METHYLBENZOYL)-PYRIDINE

Other names: 2-(2-Methylbenzoyl)-pyridine
Inchi: InChI=1S/C13H11NO/c1-10-6-2-3-7-11(10)13(15)12-8-4-5-9-14-12/h2-9H,1H3
InchiKey: GWXTVPWMINBKEI-UHFFFAOYSA-N
Formula: C13H11NO
SMILES: Cc1ccccc1C(=O)c1ccccn1
Mol. weight [g/mol]: 197.24

Physical Properties

Property code	Value	Unit	Source
hf	66.81	kJ/mol	Cheméo Relay (1.0)
hvap	85.68	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-2.65		Cheméo Relay (1.0)
logp	2.621		Crippen Method
mcvol	158.060	ml/mol	McGowan Method
tb	598.37	K	Cheméo Relay (1.0)
tc	863.88	K	Cheméo Relay (1.0)
tf	327.67	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54523783&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point