Methanone,(2-bromophenyl)-2-pyridinyl-

Other names: 2-(2-Bromobenzoyl)pyridine
Inchi: InChI=1S/C12H8BrNO/c13-10-6-2-1-5-9(10)12(15)11-7-3-4-8-14-11/h1-8H
InchiKey: HMODYVBYHZJGSW-UHFFFAOYSA-N
Formula: C12H8BrNO
SMILES: O=C(c1ccccn1)c1ccccc1Br
Mol. weight [g/mol]: 262.10
CAS: 76160-34-4

Physical Properties

Property code	Value	Unit	Source
ie	8.93	eV	NIST Webbook
log10ws	-4.36		Crippen Method
logp	3.075		Crippen Method
mcvol	161.470	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76160344&Units=SI

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume