Methanone, 2-furanylphenyl-

Inchi: InChI=1S/C11H8O2/c12-11(10-7-4-8-13-10)9-5-2-1-3-6-9/h1-8H
InchiKey: CRLNTRZMHKNJSR-UHFFFAOYSA-N
Formula: C11H8O2
SMILES: O=C(c1ccccc1)c1ccco1
Mol. weight [g/mol]: 172.18
CAS: 2689-59-0

Physical Properties

Property code	Value	Unit	Source
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-7.16		Crippen Method
logp	2.511		Crippen Method
mcvol	130.070	ml/mol	McGowan Method
tb	558.20	K	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2689590&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

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

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