

2-(p-Methoxybenzoyl)thiophene

Other names:	2-(4-Methoxybenzoyl)thiophene Methanone, (4-methoxyphenyl)-2-thienyl- p-anisyl thiophen-2-yl ketone
Inchi:	InChI=1S/C12H10O2S/c1-14-10-6-4-9(5-7-10)12(13)11-3-2-8-15-11/h2-8H,1H3
InchiKey:	KYVBFEMQEUXVQB-UHFFFAOYSA-N
Formula:	C12H10O2S
SMILES:	<chem>COc1ccc(C(=O)c2cccs2)cc1</chem>
Mol. weight [g/mol]:	218.27
CAS:	4160-63-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.988		Crippen Method
mcvol	160.510	ml/mol	McGowan Method

Sources

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=C4160638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/39-691-2/2-p-Methoxybenzoyl-thiophene.pdf>

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