

2-(Pentamethylbenzoyl)thiophene

Inchi:	InChI=1S/C16H18OS/c1-9-10(2)12(4)15(13(5)11(9)3)16(17)14-7-6-8-18-14/h6-8H,1-5H3
InchiKey:	ZGEZTRBQIJWTJL-UHFFFAOYSA-N
Formula:	C16H18OS
SMILES:	Cc1c(C)c(C)c(C(=O)c2cccs2)c(C)c1C
Mol. weight [g/mol]:	258.38
CAS:	175136-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	4.521		Crippen Method
mcvol	211.000	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C175136706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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