

2,5-Dicarboxy-3,4-diphenyl-thiophene

Inchi:	InChI=1S/C18H12O4S/c19-17(20)15-13(11-7-3-1-4-8-11)14(16(23-15)18(21)22)12-9-5-2
InchiKey:	UHMRUNRNPLYJU-UHFFFAOYSA-N
Formula:	C18H12O4S
SMILES:	O=C(O)c1sc(C(=O)O)c(-c2ccccc2)c1-c1ccccc1
Mol. weight [g/mol]:	324.35
CAS:	19799-42-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.56		Crippen Method
logp	4.479		Crippen Method
mcvol	228.730	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19799429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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