2,2':5',2''-Terthiophene

Other names:	2,2',5',2''-Terthienyl
	2,2',5',2''-terthienyl, («alpha»-erthiophene, «alpha»-terthienyl)
	2,2'-Bithiophene, 5-(2-thienyl)-
	2,2':5',2''-terthienyl
	2,2':5'2''-Terthiophene
	2,5-di-2-thienylthiophene
	«alpha»-Terthienyl
Inchi:	InChI=1S/C12H8S3/c1-3-9(13-7-1)11-5-6-12(15-11)10-4-2-8-14-10/h1-8H
InchiKey:	KXSFECAJUBPPFE-UHFFFAOYSA-N
Formula:	C12H8S3
SMILES:	c1csc(-c2ccc(-c3cccs3)s2)c1
Mol. weight [g/mol]:	248.39
CAS:	1081-34-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.95		Crippen Method
logp	5.205		Crippen Method
mcvol	170.610	ml/mol	McGowan Method
rinpol	2239.40		NIST Webbook
rinpol	2243.00		NIST Webbook
tf	365.30	K	Phase transition equilibrium of terthiophene isomers

Sources

Phase transition equilibrium of terthiophene isomers:	https://www.doi.org/10.1016/j.jct.2010.08.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1081341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point