4-Methyl-2-(3,7,11-Trimethyldodecyl) thiophene

Inchi: InChI=1S/C20H36S/c1-16(2)8-6-9-17(3)10-7-11-18(4)12-13-20-14-19(5)15-21-20/h14-18
InchiKey: UXJJRGIAVJTECT-UHFFFAOYSA-N
Formula: C20H36S
SMILES: Cc1csc(CCC(C)CCCC(C)CCCC(C)C)c1
Mol. weight [g/mol]: 308.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	7.258		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2144.00		NIST Webbook

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=U360377&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices