2-(4,8,12-Trimethyltridecyl) thiophene

Inchi: InChI=1S/C20H36S/c1-17(2)9-5-10-18(3)11-6-12-19(4)13-7-14-20-15-8-16-21-20/h8,15-1
InchiKey: BEQHRVXLXPZBRF-UHFFFAOYSA-N
Formula: C20H36S
SMILES: CC(C)CCCC(C)CCCC(C)CCCc1cccs1
Mol. weight [g/mol]: 308.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.17		Crippen Method
logp	7.340		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
rinpol	2123.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360372&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