

3-(4,8,12-Trimethyltridecyl)thiophene

Inchi: InChI=1S/C20H36S/c1-17(2)8-5-9-18(3)10-6-11-19(4)12-7-13-20-14-15-21-16-20/h14-19
InchiKey: HCUPGGLNJFUUFZ-UHFFFAOYSA-N
Formula: C20H36S
SMILES: CC(C)CCCC(C)CCCC(C)CCCc1ccsc1
Mol. weight [g/mol]: 308.56
CAS: 102037-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.17		Crippen Method
logp	7.340		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
rinpole	2138.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C102037898&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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