

Thiophene, 2-ethyl-5-dodecyl

Other names: 2-Ethyl-5-dodecylthiophene
Inchi: InChI=1S/C18H32S/c1-3-5-6-7-8-9-10-11-12-13-14-18-16-15-17(4-2)19-18/h15-16H,3-14H
InchiKey: HVSFNDSYINAMRD-UHFFFAOYSA-N
Formula: C18H32S
SMILES: CCCCCCCCCCCCc1ccc(CC)s1
Mol. weight [g/mol]: 280.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	6.774		Crippen Method
mcvol	261.370	ml/mol	McGowan Method
rinpol	2046.00		NIST Webbook
rinpol	2048.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41829&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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