

2-Thiopheneacetic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C19H28O2S/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-19(20)17-18-14-13-16-22-18/
InchiKey: WRHULFWLMAUXJM-UHFFFAOYSA-N
Formula: C19H28O2S
SMILES: CCCCCCCCCC#CCOC(=O)Cc1cccs1
Mol. weight [g/mol]: 320.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	5.368		Crippen Method
mcvol	274.300	ml/mol	McGowan Method
rinpola	2363.00		NIST Webbook
rinpola	2363.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299391&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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