

2-Thiopheneacetic acid, 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C15H20O2S/c1-4-5-7-13(10-12(2)3)17-15(16)11-14-8-6-9-18-14/h6,8-9,12-13
InchiKey:	PWPBUBHLPVWYDJ-UHFFFAOYSA-N
Formula:	C15H20O2S
SMILES:	CCC#CC(CC(C)C)OC(=O)Cc1cccs1
Mol. weight [g/mol]:	264.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	3.662		Crippen Method
mcvol	217.940	ml/mol	McGowan Method
rinpola	1761.00		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=U299387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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