

Thiophene, 2-(pentylthio)-

Other names:	1-(2-Thienyl)-1-thiahexane 2-(Pentylthio)-thiophene
Inchi:	InChI=1S/C9H14S2/c1-2-3-4-7-10-9-6-5-8-11-9/h5-6,8H,2-4,7H2,1H3
InchiKey:	PMOLPBAEMHMCKW-UHFFFAOYSA-N
Formula:	C9H14S2
SMILES:	CCCCCSc1cccs1
Mol. weight [g/mol]:	186.34
CAS:	54798-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	4.030		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
rinpol	1372.00		NIST Webbook
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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=C54798877&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
rinpol:	Non-polar retention indices

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