

# Thiophene, 2-butyl-5-hexyl-

<b>Other names:</b>	2-Butyl-5-hexylthiophene
<b>Inchi:</b>	InChI=1S/C14H24S/c1-3-5-7-8-10-14-12-11-13(15-14)9-6-4-2/h11-12H,3-10H2,1-2H3
<b>InchiKey:</b>	ALQRWUZNMBDWAU-UHFFFAOYSA-N
<b>Formula:</b>	C14H24S
<b>SMILES:</b>	CCCCCCc1ccc(CCCC)s1
<b>Mol. weight [g/mol]:</b>	224.41
<b>CAS:</b>	4806-12-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	5.214		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinsol	1679.00		NIST Webbook
rinsol	1679.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4806126&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4806126&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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