

# Thiophene, 2-heptyl-

<b>Other names:</b>	2-Heptylthiophene 2-n-Heptylthiophene
<b>Inchi:</b>	InChI=1S/C11H18S/c1-2-3-4-5-6-8-11-9-7-10-12-11/h7,9-10H,2-6,8H2,1H3
<b>InchiKey:</b>	FGGZOCMVJAJPMH-UHFFFAOYSA-N
<b>Formula:</b>	C11H18S
<b>SMILES:</b>	CCCCCCCc1cccs1
<b>Mol. weight [g/mol]:</b>	182.33
<b>CAS:</b>	18794-78-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	4.261		Crippen Method
mcpol	162.740	ml/mol	McGowan Method
ripol	1379.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1684.00		NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54959e+01
Coeff. B	-4.65366e+03
Coeff. C	-8.60850e+01
Temperature range (K), min.	392.08
Temperature range (K), max.	543.02

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C18794780&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18794780&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

# 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>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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