

# 2-n-Heptylfuran

<b>Other names:</b>	2-Heptylfuran Furan, 2-heptyl-
<b>Inchi:</b>	InChI=1S/C11H18O/c1-2-3-4-5-6-8-11-9-7-10-12-11/h7,9-10H,2-6,8H2,1H3
<b>InchiKey:</b>	BHTUFJXTYNLISA-UHFFFAOYSA-N
<b>Formula:</b>	C11H18O
<b>SMILES:</b>	CCCCCCCc1ccco1
<b>Mol. weight [g/mol]:</b>	166.26
<b>CAS:</b>	3777-71-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.10		Crippen Method
logp	3.792		Crippen Method
mcpvol	152.260	ml/mol	McGowan Method
ripol	1184.00		NIST Webbook
ripol	1182.00		NIST Webbook
ripol	1182.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1182.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1429.00		NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42324e+01
Coeff. B	-3.91069e+03
Coeff. C	-7.08790e+01
Temperature range (K), min.	351.32
Temperature range (K), max.	509.25

## Sources

The Yaws Handbook of Vapor

Pressure:  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C3777717&Units=SI>

## 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>ripol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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