

Thiophene, 2-hexyl-

Other names:	2-Hexylthiophene 2-n-Hexylthiophene
Inchi:	InChI=1S/C10H16S/c1-2-3-4-5-7-10-8-6-9-11-10/h6,8-9H,2-5,7H2,1H3
InchiKey:	QZVHYFUVMQIGGM-UHFFFAOYSA-N
Formula:	C10H16S
SMILES:	CCCCCCc1cccs1
Mol. weight [g/mol]:	168.30
CAS:	18794-77-9

Physical Properties

Property code	Value	Unit	Source
hvap	56.40 ± 1.30	kJ/mol	NIST Webbook
log10ws	-3.71		Crippen Method
logp	3.871		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
ripol	1274.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1245.00		NIST Webbook
ripol	1245.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1544.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1532.00		NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54164e+01
Coeff. B	-4.47772e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	376.72
Temperature range (K), max.	523.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18794779&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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