

3-Hexylthiophene

Inchi:	InChI=1S/C10H16S/c1-2-3-4-5-6-10-7-8-11-9-10/h7-9H,2-6H2,1H3
InchiKey:	JEDHEMYZURJGRQ-UHFFFAOYSA-N
Formula:	C10H16S
SMILES:	CCCCCCc1ccsc1
Mol. weight [g/mol]:	168.30
CAS:	1693-86-3

Physical Properties

Property code	Value	Unit	Source
hvap	58.50 ± 1.30	kJ/mol	NIST Webbook
log10ws	-3.71		Crippen Method
logp	3.871		Crippen Method
mvol	148.650	ml/mol	McGowan Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56026e+01
Coeff. B	-4.54880e+03
Coeff. C	-8.13040e+01
Temperature range (K), min.	378.32
Temperature range (K), max.	523.32

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

McGowan Method:

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

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

<http://link.springer.com/article/10.1007/BF02311772>

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_{vap}:	Vapor pressure

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