

3-n-Hexadecylthiophene

Other names:	3-Hexadecylthiophene
Inchi:	InChI=1S/C20H36S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-17-18-21-19-20/h17-19
InchiKey:	FRVZSODZVJPMKO-UHFFFAOYSA-N
Formula:	C20H36S
SMILES:	CCCCCCCCCCCCCCCCc1ccsc1
Mol. weight [g/mol]:	308.56
CAS:	---

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.89		Crippen Method
logp	7.772		Crippen Method
mvol	289.550	ml/mol	McGowan Method
rinpol	2303.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2349.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45052e+01
Coeff. B	-5.22328e+03
Coeff. C	-1.18778e+02
Temperature range (K), min.	486.16
Temperature range (K), max.	686.92

Sources

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

Crippen Method:	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=U360375&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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

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