

2-Tetradecylthiophene

Other names:	Thiophene, 2-tetradecyl
Inchi:	InChI=1S/C18H32S/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-16-14-17-19-18/h14,16-17H,2
InchiKey:	HZZUFNXZYKMRBE-UHFFFAOYSA-N
Formula:	C18H32S
SMILES:	CCCCCCCCCCCCCc1cccs1
Mol. weight [g/mol]:	280.51
CAS:	---

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Crippen Method
logp	6.992		Crippen Method
mcvol	261.370	ml/mol	McGowan Method
rinpol	2087.30		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2087.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45707e+01
Coeff. B	-5.06843e+03
Coeff. C	-1.12106e+02
Temperature range (K), min.	467.15
Temperature range (K), max.	659.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41865&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.chemeo.com/doc/models/crippen_log10ws

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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