Thiophene, 2-octyl-

Other names:	2-Octylthiophene
	2-n-Octylthiophene
Inchi:	InChI=1S/C12H20S/c1-2-3-4-5-6-7-9-12-10-8-11-13-12/h8,10-11H,2-7,9H2,1H3
InchiKey:	GIFWAJGKWIDXMY-UHFFFAOYSA-N
Formula:	C12H20S
SMILES:	CCCCCCCCc1cccs1
Mol. weight [g/mol]:	196.35
CAS:	880-36-4

Physical Properties

Property code	Value	Unit	Source
hvap	65.40 ± 1.40	kJ/mol	NIST Webbook
log10ws	-4.54		Crippen Method
logp	4.651		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
rinpol	1463.00		NIST Webbook
ripol	1780.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53338e+01
Coeff. B	-4.72581e+03
Coeff. C	-9.03940e+01
Temperature range (K), min.	404.48
Temperature range (K), max.	561.92

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C880364&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/ci990307l
Crippen Method:	https://www.chemeo.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