

3-Octylthiophene

Inchi: InChI=1S/C12H20S/c1-2-3-4-5-6-7-8-12-9-10-13-11-12/h9-11H,2-8H2,1H3
InchiKey: WQYWXQCOYRZFAV-UHFFFAOYSA-N
Formula: C12H20S
SMILES: CCCCCCCCc1ccsc1
Mol. weight [g/mol]: 196.35
CAS: 65016-62-8

Physical Properties

Property code	Value	Unit	Source
hvap	67.60 ± 1.50	kJ/mol	NIST Webbook
log10ws	-4.54		Crippen Method
logp	4.651		Crippen Method
mvol	176.830	ml/mol	McGowan Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55067e+01
Coeff. B	-4.79599e+03
Coeff. C	-9.09500e+01
Temperature range (K), min.	406.08
Temperature range (K), max.	561.37

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65016628&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

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

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