

Thiophene, 3-propyl-

Other names:	3-Propylthiophene
Inchi:	InChI=1S/C7H10S/c1-2-3-7-4-5-8-6-7/h4-6H,2-3H2,1H3
InchiKey:	QZNFMRMXKQCIPQY-UHFFFAOYSA-N
Formula:	C7H10S
SMILES:	CCCC1ccsc1
Mol. weight [g/mol]:	126.22
CAS:	1518-75-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Crippen Method
logp	2.701		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	946.00		NIST Webbook
rinpol	945.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44880e+01
Coeff. B	-3.63006e+03
Coeff. C	-6.47400e+01
Temperature range (K), min.	320.37
Temperature range (K), max.	460.32

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=C1518758&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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