

3-Butylthiophene

Other names:	Thiophene, 3-butyl
Inchi:	InChI=1S/C8H12S/c1-2-3-4-8-5-6-9-7-8/h5-7H,2-4H2,1H3
InchiKey:	KPOCSQCZXMATFR-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CCCCc1ccsc1
Mol. weight [g/mol]:	140.25
CAS:	34722-01-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	3.091		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1054.00		NIST Webbook
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52856e+01
Coeff. B	-4.13102e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	343.12
Temperature range (K), max.	481.86

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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=C34722015&Units=SI>

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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