

Thiophene, 2-butyl-

Other names:	2-Butylthiophene 2-n-Butylthiophene
Inchi:	InChI=1S/C8H12S/c1-2-3-5-8-6-4-7-9-8/h4,6-7H,2-3,5H2,1H3
InchiKey:	MNDZHERKKXUTOE-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CCCCc1cccs1
Mol. weight [g/mol]:	140.25
CAS:	1455-20-5

Physical Properties

Property code	Value	Unit	Source
ie	8.50 ± 0.20	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	3.091		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1065.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1045.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1351.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52375e+01
Coeff. B	-4.11388e+03
Coeff. C	-6.75430e+01
Temperature range (K), min.	342.72
Temperature range (K), max.	482.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1455205&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

ie:	Ionization energy
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

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