

Pyridine, 3-butyl-

Other names:	1-(3-Pyridyl)butane 3-Butylpyridine 3-n-Butylpyridine
Inchi:	InChI=1S/C9H13N/c1-2-3-5-9-6-4-7-10-8-9/h4,6-8H,2-3,5H2,1H3
InchiKey:	QSNMFWFDOFQASV-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCCCc1ccncc1
Mol. weight [g/mol]:	135.21
CAS:	539-32-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.424		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1101.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1101.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	479.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.70	K	1.00	NIST Webbook
tbrp	355.00	K	0.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48014e+01
Coeff. B	-4.12599e+03
Coeff. C	-7.45200e+01
Temperature range (K), min.	358.80
Temperature range (K), max.	509.29

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C539322&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.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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