

Piperidine, 1-butyl-

Other names:	1-Butylpiperidine N-Butylpiperidine
Inchi:	InChI=1S/C9H19N/c1-2-3-7-10-8-5-4-6-9-10/h2-9H2,1H3
InchiKey:	AXWLKJWVMMAxBD-UHFFFAOYSA-N
Formula:	C9H19N
SMILES:	CCCCN1CCCCC1
Mol. weight [g/mol]:	141.25
CAS:	4945-48-6

Physical Properties

Property code	Value	Unit	Source
chl	-6085.20 ± 8.50	kJ/mol	NIST Webbook
hfl	-171.80 ± 8.50	kJ/mol	NIST Webbook
hvap	48.90 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.05		Crippen Method
logp	2.272		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
rinpol	1025.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1147.00		NIST Webbook
tb	449.15 ± 2.00	K	NIST Webbook
tb	448.95 ± 0.40	K	NIST Webbook
tb	445.15 ± 5.00	K	NIST Webbook
tb	442.65 ± 3.00	K	NIST Webbook
tb	450.15 ± 2.00	K	NIST Webbook
tb	449.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	49.20 ± 0.20	kJ/mol	294.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45266e+01
Coeff. B	-3.78480e+03
Coeff. C	-6.60140e+01
Temperature range (K), min.	301.15
Temperature range (K), max.	476.73

Sources

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=C4945486&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

Legend

chl:	Standard liquid enthalpy of combustion
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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