

Pyridine, 4-propyl-

Other names:	4-Propylpyridine 4-n-Propylpyridine
Inchi:	InChI=1S/C8H11N/c1-2-3-8-4-6-9-7-5-8/h4-7H,2-3H2,1H3
InchiKey:	JAWZAONCXMJLFT-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1ccncc1
Mol. weight [g/mol]:	121.18
CAS:	1122-81-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	2.034		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
rinpol	1034.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1049.60		NIST Webbook
rinpol	1032.30		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1032.30		NIST Webbook
rinpol	1032.30		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	458.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	47.80	kJ/mol	409.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47512e+01
Coeff. B	-3.94864e+03
Coeff. C	-6.85160e+01
Temperature range (K), min.	341.52
Temperature range (K), max.	486.81

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122812&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/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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