

Pyridine, 3-propyl-

Other names:	3-Propylpyridine 1-(3-Pyridyl)propane 3-(n-Propyl)pyridine Pyridine, 5-propyl
Inchi:	InChI=1S/C8H11N/c1-2-4-8-5-3-6-9-7-8/h3,5-7H,2,4H2,1H3
InchiKey:	MLAXEZHEGARMPE-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCCC1CCCCN1
Mol. weight [g/mol]:	121.18
CAS:	4673-31-8

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	1019.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1018.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1457.00		NIST Webbook
ripol	1457.00		NIST Webbook
ripol	1460.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	49.90	kJ/mol	400.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4673318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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