

# Quinoline, 2-propyl-

<b>Other names:</b>	2-Propylquinoline
<b>Inchi:</b>	InChI=1S/C12H13N/c1-2-5-11-9-8-10-6-3-4-7-12(10)13-11/h3-4,6-9H,2,5H2,1H3
<b>InchiKey:</b>	IZXJPGLOYDHRM-UHFFFAOYSA-N
<b>Formula:</b>	C12H13N
<b>SMILES:</b>	CCCc1ccc2ccccc2n1
<b>Mol. weight [g/mol]:</b>	171.24
<b>CAS:</b>	1613-32-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.187		Crippen Method
mcvol	146.700	ml/mol	McGowan Method
ripol	1472.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2040.00		NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43268e+01
Coeff. B	-4.48426e+03

Coeff. C	-9.74910e+01
Temperature range (K), min.	416.90
Temperature range (K), max.	594.90

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613327&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613327&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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