

# 9H-Pyrido[3,4-b]indole, 1-methyl-

<b>Other names:</b>	1-Methyl-2-carboline 1-Methyl-9H-pyrid(3,4-b)indole 1-Methyl-9H-pyrido[3,4-b]indole 1-Methyl-«beta»-carboline 1-Methyl-Â«betaÂ»-carboline 1-Methylnorharman Aribin Aribine Harman Harmane Locuturin Locuturine Loturine NSC 54439 Passiflorin Pyridobindole, L-methyl-
<b>Inchi:</b>	InChI=1S/C12H10N2/c1-8-12-10(6-7-13-8)9-4-2-3-5-11(9)14-12/h2-7,14H,1H3
<b>InchiKey:</b>	PSFDQSOCUJVVGf-UHFFFAOYSA-N
<b>Formula:</b>	C12H10N2
<b>SMILES:</b>	<chem>Cc1nccc2c1[nH]c1cccc12</chem>
<b>Mol. weight [g/mol]:</b>	182.22
<b>CAS:</b>	486-84-0

## Physical Properties

Property code	Value	Unit	Source
ie	7.83 ± 0.06	eV	NIST Webbook
log10ws	-3.79		Aqueous Solubility Prediction Method
logp	2.543		Crippen Method
mcvol	141.520	ml/mol	McGowan Method
rinpol	2000.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1975.00		NIST Webbook

rinp0l	1975.00		NIST Webbook
tf	509.65	K	Aqueous Solubility Prediction Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.20	kJ/mol	509.90	NIST Webbook

## Sources

<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=C486840&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C486840&amp;Units=SI</a>
<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>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>

## Legend

<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>ie:</b>	Ionization energy
<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>rinp0l:</b>	Non-polar retention indices
<b>tf:</b>	Normal melting (fusion) point

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