

# Modaline

<b>Other names:</b>	2-Methyl-3-piperidinopyrazine
<b>Inchi:</b>	InChI=1S/C10H15N3/c1-9-10(12-6-5-11-9)13-7-3-2-4-8-13/h5-6H,2-4,7-8H2,1H3
<b>InchiKey:</b>	BJHCGMHPEKLROM-UHFFFAOYSA-N
<b>Formula:</b>	C10H15N3
<b>SMILES:</b>	Cc1nccnc1N1CCCCC1
<b>Mol. weight [g/mol]:</b>	177.25
<b>CAS:</b>	2856-74-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	1.775		Crippen Method
mcvol	147.080	ml/mol	McGowan Method
ripol	1465.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	2004.00		NIST Webbook
ripol	2015.00		NIST Webbook
ripol	2027.00		NIST Webbook
ripol	1956.00		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=C2856748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2856748&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>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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