

# C13H13NO

<b>Inchi:</b>	InChI=1S/C13H13NO/c14-9-11-7-4-8-12(13(11)15)10-5-2-1-3-6-10/h1-3,5-6,11-12H,4,7-
<b>InchiKey:</b>	IKVQMASZSHOPRA-UHFFFAOYSA-N
<b>Formula:</b>	C13H13NO
<b>SMILES:</b>	N#CC1CCCC(c2ccccc2)C1=O
<b>Mol. weight [g/mol]:</b>	199.25
<b>CAS:</b>	13658-18-9

## Physical Properties

Property code	Value	Unit	Source
gf	198.32	kJ/mol	Joback Method
hf	-13.96	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	61.65	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.663		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
tb	708.30	K	Joback Method
tc	970.41	K	Joback Method
tf	399.04	K	Joback Method
vc	0.621	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.48	J/mol×K	708.30	Joback Method
cpg	469.62	J/mol×K	751.98	Joback Method
cpg	485.26	J/mol×K	795.67	Joback Method
cpg	499.40	J/mol×K	839.35	Joback Method
cpg	512.07	J/mol×K	883.04	Joback Method
cpg	523.27	J/mol×K	926.72	Joback Method
cpg	533.03	J/mol×K	970.41	Joback Method

# 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=C13658189&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13658189&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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