

# O-phenethidine, 5-chloro

<b>Inchi:</b>	InChI=1S/C8H10ClNO/c1-2-11-8-4-3-6(9)5-7(8)10/h3-5H,2,10H2,1H3
<b>InchiKey:</b>	UZEGGYTUIIXOIX-UHFFFAOYSA-N
<b>Formula:</b>	C8H10ClNO
<b>SMILES:</b>	CCOc1ccc(Cl)cc1N
<b>Mol. weight [g/mol]:</b>	171.62
<b>CAS:</b>	15793-48-3

## Physical Properties

Property code	Value	Unit	Source
gf	59.15	kJ/mol	Joback Method
hf	-109.03	kJ/mol	Joback Method
hfus	20.32	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.321		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	551.46	K	Joback Method
tc	779.29	K	Joback Method
tf	366.79	K	Joback Method
vc	0.471	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.01	J/mol×K	551.46	Joback Method
cpg	286.31	J/mol×K	589.43	Joback Method
cpg	296.99	J/mol×K	627.40	Joback Method
cpg	307.04	J/mol×K	665.38	Joback Method
cpg	316.49	J/mol×K	703.35	Joback Method
cpg	325.33	J/mol×K	741.32	Joback Method
cpg	333.58	J/mol×K	779.29	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15793483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15793483&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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