

# Hydroxyamitryptiline

<b>Inchi:</b>	InChI=1S/C20H23NO/c1-21(2)13-5-8-19-18-7-4-3-6-15(18)9-10-16-11-12-17(22)14-20(1)
<b>InchiKey:</b>	GSCNHQHCSDAANR-UWVJOHFNSA-N
<b>Formula:</b>	C20H23NO
<b>SMILES:</b>	CN(C)CCC=C1c2ccccc2CCc2ccc(O)cc21
<b>Mol. weight [g/mol]:</b>	293.40

## Physical Properties

Property code	Value	Unit	Source
gf	393.16	kJ/mol	Joback Method
hf	53.38	kJ/mol	Joback Method
hfus	41.05	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.874		Crippen Method
mvol	245.830	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	2309.00		NIST Webbook
tb	831.43	K	Joback Method
tc	1070.04	K	Joback Method
tf	569.77	K	Joback Method
vc	0.865	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.12	J/mol×K	831.43	Joback Method
cpg	757.73	J/mol×K	871.20	Joback Method
cpg	773.61	J/mol×K	910.97	Joback Method
cpg	788.97	J/mol×K	950.74	Joback Method
cpg	804.00	J/mol×K	990.51	Joback Method
cpg	818.91	J/mol×K	1030.27	Joback Method
cpg	833.89	J/mol×K	1070.04	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R21920&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R21920&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>

# 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<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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