

# Amprotropine

<b>Inchi:</b>	InChI=1S/C18H29NO3/c1-5-19(6-2)13-18(3,4)14-22-17(21)16(12-20)15-10-8-7-9-11-15/
<b>InchiKey:</b>	ORXLOAFNULMXBG-UHFFFAOYSA-N
<b>Formula:</b>	C18H29NO3
<b>SMILES:</b>	CCN(CC)CC(C)(C)COC(=O)C(CO)c1ccccc1
<b>Mol. weight [g/mol]:</b>	307.43
<b>CAS:</b>	148-32-3

## Physical Properties

Property code	Value	Unit	Source
gf	-46.47	kJ/mol	Joback Method
hf	-521.85	kJ/mol	Joback Method
hfus	35.38	kJ/mol	Joback Method
hvap	84.13	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.674		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		NIST Webbook
tb	815.16	K	Joback Method
tc	1012.28	K	Joback Method
tf	471.91	K	Joback Method
vc	0.980	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.15	J/mol×K	815.16	Joback Method
cpg	836.49	J/mol×K	848.01	Joback Method
cpg	850.86	J/mol×K	880.87	Joback Method
cpg	864.30	J/mol×K	913.72	Joback Method
cpg	876.88	J/mol×K	946.57	Joback Method
cpg	888.67	J/mol×K	979.43	Joback Method
cpg	899.71	J/mol×K	1012.28	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C148323&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C148323&amp;Units=SI</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>hvp:</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>rinp:</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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