

# PROPAFENONE-H2O, AC

<b>Inchi:</b>	InChI=1S/C23H27NO3/c1-3-16-24(19(2)25)17-9-18-27-23-13-8-7-12-21(23)22(26)15-14
<b>InchiKey:</b>	PHFPUXKZVRGKNW-GIJQJNRQSA-N
<b>Formula:</b>	C23H27NO3
<b>SMILES:</b>	CCCN(CC=COc1cccc1C(=O)CCc1cccc1)C(C)=O
<b>Mol. weight [g/mol]:</b>	365.47

## Physical Properties

Property code	Value	Unit	Source
gf	186.13	kJ/mol	Joback Method
hf	-229.09	kJ/mol	Joback Method
hfus	50.63	kJ/mol	Joback Method
hvap	89.91	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.653		Crippen Method
mcvol	302.100	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
tb	930.74	K	Joback Method
tc	1155.87	K	Joback Method
tf	563.81	K	Joback Method
vc	1.135	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.27	J/molxK	930.74	Joback Method
cpg	958.13	J/molxK	968.26	Joback Method
cpg	971.86	J/molxK	1005.78	Joback Method
cpg	984.58	J/molxK	1043.31	Joback Method
cpg	996.36	J/molxK	1080.83	Joback Method
cpg	1007.31	J/molxK	1118.35	Joback Method
cpg	1017.52	J/molxK	1155.87	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=R255355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R255355&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>mcvol:</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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