

# protoanemonin

**Inchi:** InChI=1S/C10H8O4/c11-7-1-3-9(13-7)5-6-10(9)4-2-8(12)14-10/h1-4H,5-6H2  
**InchiKey:** JLUQTCXCAFSSLD-UHFFFAOYSA-N  
**Formula:** C10H8O4  
**SMILES:** O=C1C=CC2(CCC23C=CC(=O)O3)O1  
**Mol. weight [g/mol]:** 192.17  
**CAS:** 90921-11-2

## Physical Properties

Property code	Value	Unit	Source
gf	-181.50	kJ/mol	Joback Method
hf	-422.83	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.484		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
tb	654.24	K	Joback Method
tc	937.51	K	Joback Method
tf	488.86	K	Joback Method
vc	0.468	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.72	J/molxK	654.24	Joback Method
cpg	366.28	J/molxK	701.45	Joback Method
cpg	380.23	J/molxK	748.66	Joback Method
cpg	394.01	J/molxK	795.87	Joback Method
cpg	408.07	J/molxK	843.09	Joback Method
cpg	422.85	J/molxK	890.30	Joback Method
cpg	438.81	J/molxK	937.51	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=C90921112&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90921112&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>

# 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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