

# Pentyl angelate

<b>Inchi:</b>	InChI=1S/C10H18O2/c1-4-6-7-8-12-10(11)9(3)5-2/h5H,4,6-8H2,1-3H3/b9-5-
<b>InchiKey:</b>	XJWDRSSGOHXOLQ-UITAMQMPSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	CC=C(C)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	170.25

## Physical Properties

Property code	Value	Unit	Source
gf	-128.93	kJ/mol	Joback Method
hf	-387.10	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1162.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1162.00		NIST Webbook
tb	508.53	K	Joback Method
tc	691.44	K	Joback Method
tf	255.58	K	Joback Method
vc	0.601	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.59	J/molxK	508.53	Joback Method
cpg	364.62	J/molxK	539.01	Joback Method
cpg	378.03	J/molxK	569.50	Joback Method
cpg	390.86	J/molxK	599.98	Joback Method
cpg	403.11	J/molxK	630.47	Joback Method
cpg	414.81	J/molxK	660.95	Joback Method
cpg	425.96	J/molxK	691.44	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R288390&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R288390&amp;Units=SI</a>
<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.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>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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