

# ipsdienyl acetate

<b>Inchi:</b>	InChI=1S/C12H18O2/c1-6-10(4)8-12(7-9(2)3)14-11(5)13/h6-7,12H,1,4,8H2,2-3,5H3
<b>InchiKey:</b>	ZTRGTWAVPUGVON-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O2
<b>SMILES:</b>	<chem>C=CC(=C)CC(C=C(C)C)OC(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	194.27

## Physical Properties

Property code	Value	Unit	Source
gf	52.60	kJ/mol	Joback Method
hf	-192.59	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.017		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
ripol	1594.00		NIST Webbook
tb	547.09	K	Joback Method
tc	739.96	K	Joback Method
tf	245.64	K	Joback Method
vc	0.669	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.18	J/molxK	547.09	Joback Method
cpg	421.19	J/molxK	579.23	Joback Method
cpg	435.43	J/molxK	611.38	Joback Method
cpg	448.94	J/molxK	643.52	Joback Method
cpg	461.74	J/molxK	675.67	Joback Method
cpg	473.87	J/molxK	707.81	Joback Method
cpg	485.35	J/molxK	739.96	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.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=R494030&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R494030&amp;Units=SI</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ri<sub>npol</sub>:</b>	Non-polar retention indices
<b>ri<sub>pol</sub>:</b>	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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