

# Sabinol isovalerate

<b>Inchi:</b>	InChI=1S/C15H24O2/c1-9(2)6-14(16)17-13-8-15(10(3)4)7-12(15)11(13)5/h9-10,12-13H,5
<b>InchiKey:</b>	PHHDSFRGHUTRPK-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	<chem>C=C1C(OC(=O)CC(C)C)CC2(C(C)C)CC12</chem>
<b>Mol. weight [g/mol]:</b>	236.35
<b>CAS:</b>	5281-02-7

## Physical Properties

Property code	Value	Unit	Source
gf	-2.00	kJ/mol	Joback Method
hf	-383.55	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.567		Crippen Method
mvol	203.630	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1514.60		NIST Webbook
tb	626.22	K	Joback Method
tc	827.69	K	Joback Method
tf	370.19	K	Joback Method
vc	0.782	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.31	J/mol×K	626.22	Joback Method
cpg	588.78	J/mol×K	659.80	Joback Method
cpg	606.29	J/mol×K	693.38	Joback Method
cpg	622.97	J/mol×K	726.96	Joback Method
cpg	638.96	J/mol×K	760.54	Joback Method
cpg	654.35	J/mol×K	794.11	Joback Method
cpg	669.29	J/mol×K	827.69	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=C5281027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5281027&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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