

# Aristol-1(10)-en-9-yl isovalerate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H32O2/c1-12(2)10-17(21)22-16-11-15-18(19(15,4)5)20(6)13(3)8-7-9-14(16)H

ZHVACGRFWGEIFE-UHFFFAOYSA-N

C20H32O2

CC(C)CC(=O)OC1CC2C(C2(C)C)C2(C)C1=CCCC2C

304.47

## Physical Properties

Property code	Value	Unit	Source
gf	25.43	kJ/mol	Joback Method
hf	-484.36	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.983		Crippen Method
mcvol	263.220	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2052.70		NIST Webbook
rinpol	2052.70		NIST Webbook
tb	752.22	K	Joback Method
tc	967.41	K	Joback Method
tf	467.46	K	Joback Method
vc	1.008	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.31	J/molxK	752.22	Joback Method
cpg	868.49	J/molxK	788.08	Joback Method
cpg	891.11	J/molxK	823.95	Joback Method
cpg	913.42	J/molxK	859.81	Joback Method
cpg	935.66	J/molxK	895.68	Joback Method
cpg	958.08	J/molxK	931.54	Joback Method
cpg	980.93	J/molxK	967.41	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=U414306&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U414306&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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