

# Anisyl valerate

<b>Other names:</b>	Anisyl n-valerate
<b>Inchi:</b>	InChI=1S/C13H18O3/c1-3-4-5-13(14)16-10-11-6-8-12(15-2)9-7-11/h6-9H,3-5,10H2,1-2H
<b>InchiKey:</b>	VSOLIGQDEYVGKS-UHFFFAOYSA-N
<b>Formula:</b>	C13H18O3
<b>SMILES:</b>	CCCCC(=O)OCc1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	222.28

## Physical Properties

Property code	Value	Unit	Source
gf	-177.56	kJ/mol	Joback Method
hf	-463.61	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.929		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	627.21	K	Joback Method
tc	829.16	K	Joback Method
tf	369.60	K	Joback Method
vc	0.698	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.42	J/molxK	627.21	Joback Method
cpg	537.75	J/molxK	795.50	Joback Method
cpg	525.67	J/molxK	761.85	Joback Method
cpg	512.81	J/molxK	728.19	Joback Method

cpg	499.15	J/mol×K	694.53	Joback Method
cpg	484.69	J/mol×K	660.87	Joback Method
cpg	549.04	J/mol×K	829.16	Joback Method
dvisc	0.0001313	Paxs	627.21	Joback Method
dvisc	0.0001661	Paxs	584.28	Joback Method
dvisc	0.0002181	Paxs	541.34	Joback Method
dvisc	0.0003002	Paxs	498.41	Joback Method
dvisc	0.0004388	Paxs	455.47	Joback Method
dvisc	0.0006941	Paxs	412.54	Joback Method
dvisc	0.0012215	Paxs	369.60	Joback Method

## Sources

<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=R181818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R181818&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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