

# (E)-Nuciferyl isovalerate

<b>Inchi:</b>	InChI=1S/C20H30O2/c1-16(2)14-20(21)22-15-18(4)8-6-5-7-9-19-12-10-17(3)11-13-19/h
<b>InchiKey:</b>	LBFPTRSLQDXDHA-QGMBQPNBSA-N
<b>Formula:</b>	C20H30O2
<b>SMILES:</b>	CC(=CCCCC1ccc(C)cc1)COC(=O)CC(C)C
<b>Mol. weight [g/mol]:</b>	302.45

## Physical Properties

Property code	Value	Unit	Source
gf	55.61	kJ/mol	Joback Method
hf	-373.72	kJ/mol	Joback Method
hfus	39.36	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.243		Crippen Method
mcvol	272.040	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	768.55	K	Joback Method
tc	969.63	K	Joback Method
tf	392.22	K	Joback Method
vc	1.046	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.80	J/molxK	768.55	Joback Method
cpg	819.94	J/molxK	802.06	Joback Method
cpg	837.00	J/molxK	835.58	Joback Method
cpg	853.04	J/molxK	869.09	Joback Method
cpg	868.10	J/molxK	902.60	Joback Method
cpg	882.24	J/molxK	936.11	Joback Method
cpg	895.49	J/molxK	969.63	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=R233088&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233088&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>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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