

# ( Z)-nuciferyl propanoate

<b>Inchi:</b>	InChI=1S/C17H24O2/c1-4-17(18)19-13-14(2)9-8-10-15(3)16-11-6-5-7-12-16/h5-7,9,11-1
<b>InchiKey:</b>	KHAFAJWRDKUPHE-ZROIWOOFSA-N
<b>Formula:</b>	C17H24O2
<b>SMILES:</b>	CCC(=O)OCC(C)=CCCC(C)c1cccc1
<b>Mol. weight [g/mol]:</b>	260.37

## Physical Properties

Property code	Value	Unit	Source
gf	39.98	kJ/mol	Joback Method
hf	-300.33	kJ/mol	Joback Method
hfus	31.98	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.470		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinsol	1875.00		NIST Webbook
tb	694.93	K	Joback Method
tc	901.07	K	Joback Method
tf	345.89	K	Joback Method
vc	0.878	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.49	J/mol×K	694.93	Joback Method
cpg	650.04	J/mol×K	729.29	Joback Method
cpg	666.53	J/mol×K	763.64	Joback Method
cpg	682.01	J/mol×K	798.00	Joback Method
cpg	696.52	J/mol×K	832.36	Joback Method
cpg	710.11	J/mol×K	866.72	Joback Method
cpg	722.83	J/mol×K	901.07	Joback Method

# Sources

<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=R420396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R420396&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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