

# (E)-Nuciferyl acetate

<b>Inchi:</b>	InChI=1S/C17H24O2/c1-14-9-11-17(12-10-14)8-6-4-5-7-15(2)13-19-16(3)18/h7,9-12H,4-
<b>InchiKey:</b>	BWLPFSJVSUPCNH-VIZOYTHASA-N
<b>Formula:</b>	C17H24O2
<b>SMILES:</b>	CC(=O)OCC(C)=CCCCc1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	260.37

## Physical Properties

Property code	Value	Unit	Source
gf	32.79	kJ/mol	Joback Method
hf	-306.52	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	65.57	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.217		Crippen Method
mvol	229.770	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	700.35	K	Joback Method
tc	903.88	K	Joback Method
tf	373.41	K	Joback Method
vc	0.884	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.58	J/mol×K	700.35	Joback Method
cpg	648.67	J/mol×K	734.27	Joback Method
cpg	664.77	J/mol×K	768.19	Joback Method
cpg	679.92	J/mol×K	802.12	Joback Method
cpg	694.16	J/mol×K	836.04	Joback Method
cpg	707.53	J/mol×K	869.96	Joback Method
cpg	720.07	J/mol×K	903.88	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=R233593&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233593&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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