

# (Z)-Nuciferyl formate

<b>Inchi:</b>	InChI=1S/C16H22O2/c1-14-8-10-16(11-9-14)7-5-3-4-6-15(2)12-18-13-17/h6,8-11,13H,3-
<b>InchiKey:</b>	LIGLXUWLWGOJKZ-UUASQNMZSA-N
<b>Formula:</b>	C16H22O2
<b>SMILES:</b>	CC(=CCCCC1ccc(C)cc1)COC=O
<b>Mol. weight [g/mol]:</b>	246.34

## Physical Properties

Property code	Value	Unit	Source
gf	53.77	kJ/mol	Joback Method
hf	-258.88	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	63.32	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.827		Crippen Method
mvol	215.680	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rmpol	1742.00		NIST Webbook
rmpol	1742.00		NIST Webbook
tb	672.26	K	Joback Method
tc	874.43	K	Joback Method
tf	354.21	K	Joback Method
vc	0.840	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.18	J/mol×K	672.26	Joback Method
cpg	593.64	J/mol×K	705.95	Joback Method
cpg	609.16	J/mol×K	739.65	Joback Method
cpg	623.77	J/mol×K	773.34	Joback Method
cpg	637.52	J/mol×K	807.04	Joback Method
cpg	650.46	J/mol×K	840.73	Joback Method
cpg	662.60	J/mol×K	874.43	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=R233355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233355&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>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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