

# (Z)-Nuciferyl propionate

<b>Inchi:</b>	InChI=1S/C18H26O2/c1-5-18(19)20-13-15(3)7-6-8-16(4)17-11-9-14(2)10-12-17/h7,9-12,
<b>InchiKey:</b>	MGDICXSXKLAPND-CHHVJCJISA-N
<b>Formula:</b>	C18H26O2
<b>SMILES:</b>	CCC(=O)OCC(C)=CCCC(C)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	274.40

## Physical Properties

Property code	Value	Unit	Source
gf	38.77	kJ/mol	Joback Method
hf	-332.44	kJ/mol	Joback Method
hfus	34.18	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.778		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	722.79	K	Joback Method
tc	927.32	K	Joback Method
tf	369.68	K	Joback Method
vc	0.934	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.56	J/molxK	722.79	Joback Method
cpg	705.25	J/molxK	756.88	Joback Method
cpg	721.88	J/molxK	790.97	Joback Method
cpg	737.51	J/molxK	825.05	Joback Method
cpg	752.18	J/molxK	859.14	Joback Method
cpg	765.94	J/molxK	893.23	Joback Method
cpg	778.82	J/molxK	927.32	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R441704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R441704&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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