

# Dicyclohexyl azelate

<b>Inchi:</b>	InChI=1S/C21H36O4/c22-20(24-18-12-6-4-7-13-18)16-10-2-1-3-11-17-21(23)25-19-14-8
<b>InchiKey:</b>	WDBJAELSRFRZAG-UHFFFAOYSA-N
<b>Formula:</b>	C21H36O4
<b>SMILES:</b>	O=C(CCCCCCCC(=O)OC1CCCCC1)OC1CCCCC1
<b>Mol. weight [g/mol]:</b>	352.51
<b>CAS:</b>	18803-77-5

## Physical Properties

Property code	Value	Unit	Source
gf	-293.00	kJ/mol	Joback Method
hf	-857.73	kJ/mol	Joback Method
hfus	39.39	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.469		Crippen Method
mvol	299.910	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2554.00		NIST Webbook
rinpol	2554.00		NIST Webbook
tb	871.56	K	Joback Method
tc	1084.97	K	Joback Method
tf	485.51	K	Joback Method
vc	1.125	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.74	J/molxK	871.56	Joback Method
cpg	1044.41	J/molxK	907.13	Joback Method
cpg	1062.40	J/molxK	942.70	Joback Method
cpg	1078.74	J/molxK	978.26	Joback Method
cpg	1093.46	J/molxK	1013.83	Joback Method
cpg	1106.60	J/molxK	1049.40	Joback Method
cpg	1118.20	J/molxK	1084.97	Joback Method

dvisc	0.0009695	Paxs	485.51	Joback Method
dvisc	0.0004405	Paxs	549.85	Joback Method
dvisc	0.0002361	Paxs	614.19	Joback Method
dvisc	0.0001425	Paxs	678.53	Joback Method
dvisc	0.0000938	Paxs	742.88	Joback Method
dvisc	0.0000660	Paxs	807.22	Joback Method
dvisc	0.0000490	Paxs	871.56	Joback Method

## Sources

<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>
<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=C18803775&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18803775&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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