

# di-(1,3-Dimethylbutyl)azelate

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-16(2)14-18(5)24-20(22)12-10-8-7-9-11-13-21(23)25-19(6)15-17
<b>InchiKey:</b>	IOVULKSZXHYNBH-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CC(C)CC(C)OC(=O)CCCCCCCC(=O)OC(C)CC(C)C
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-351.66	kJ/mol	Joback Method
hf	-987.49	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.673		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rmpol	2163.00		NIST Webbook
tb	830.70	K	Joback Method
tc	1020.47	K	Joback Method
tf	410.75	K	Joback Method
vc	1.236	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.14	J/molxK	830.70	Joback Method
cpg	1051.06	J/molxK	862.33	Joback Method
cpg	1068.79	J/molxK	893.96	Joback Method
cpg	1085.37	J/molxK	925.58	Joback Method
cpg	1100.82	J/molxK	957.21	Joback Method
cpg	1115.14	J/molxK	988.84	Joback Method
cpg	1128.36	J/molxK	1020.47	Joback Method
dvisc	0.0016234	Paxs	410.75	Joback Method
dvisc	0.0005267	Paxs	480.74	Joback Method

dvisc	0.0002275	Paxs	550.73	Joback Method
dvisc	0.0001187	Paxs	620.73	Joback Method
dvisc	0.0000707	Paxs	690.72	Joback Method
dvisc	0.0000463	Paxs	760.71	Joback Method
dvisc	0.0000326	Paxs	830.70	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=R541587&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R541587&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>mccvol:</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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