

# di-(3-Methoxybutyl)azelate

<b>Inchi:</b>	InChI=1S/C19H36O6/c1-16(22-3)12-14-24-18(20)10-8-6-5-7-9-11-19(21)25-15-13-17(2)2
<b>InchiKey:</b>	OPGXSCQBKYRMPY-UHFFFAOYSA-N
<b>Formula:</b>	C19H36O6
<b>SMILES:</b>	COC(C)CCOC(=O)CCCCCCCC(=O)OCCC(C)OC
<b>Mol. weight [g/mol]:</b>	360.49

## Physical Properties

Property code	Value	Unit	Source
gf	-573.62	kJ/mol	Joback Method
hf	-1200.09	kJ/mol	Joback Method
hfus	45.87	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.654		Crippen Method
mcvol	305.190	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinsol	2342.00		NIST Webbook
tb	830.66	K	Joback Method
tc	1019.18	K	Joback Method
tf	462.67	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.42	J/molxK	830.66	Joback Method
cpg	1048.03	J/molxK	987.76	Joback Method
cpg	1035.27	J/molxK	956.34	Joback Method
cpg	1021.33	J/molxK	924.92	Joback Method
cpg	1006.21	J/molxK	893.50	Joback Method
cpg	989.90	J/molxK	862.08	Joback Method
cpg	1059.59	J/molxK	1019.18	Joback Method
dvisc	0.0000289	Paxs	830.66	Joback Method
dvisc	0.0000392	Paxs	769.33	Joback Method

dvisc	0.0000559	Paxs	708.00	Joback Method
dvisc	0.0000853	Paxs	646.66	Joback Method
dvisc	0.0001422	Paxs	585.33	Joback Method
dvisc	0.0002674	Paxs	524.00	Joback Method
dvisc	0.0005940	Paxs	462.67	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R542213&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R542213&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.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>

## 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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