

# di-(2-Methoxybutyl)adipate

<b>Inchi:</b>	InChI=1S/C16H30O6/c1-5-13(19-3)11-21-15(17)9-7-8-10-16(18)22-12-14(6-2)20-4/h13-1
<b>InchiKey:</b>	ZIIXQOIKXUYFAM-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O6
<b>SMILES:</b>	CCC(COC(=O)CCCCC(=O)OCC(CC)OC)OC
<b>Mol. weight [g/mol]:</b>	318.41

## Physical Properties

Property code	Value	Unit	Source
gf	-598.88	kJ/mol	Joback Method
hf	-1138.17	kJ/mol	Joback Method
hfus	38.10	kJ/mol	Joback Method
hvap	73.57	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.483		Crippen Method
mcvol	262.920	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	1746.00		NIST Webbook
tb	762.02	K	Joback Method
tc	944.23	K	Joback Method
tf	428.86	K	Joback Method
vc	1.004	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.68	J/molxK	762.02	Joback Method
cpg	867.47	J/molxK	913.86	Joback Method
cpg	854.84	J/molxK	883.50	Joback Method
cpg	841.24	J/molxK	853.13	Joback Method
cpg	826.67	J/molxK	822.76	Joback Method
cpg	811.15	J/molxK	792.39	Joback Method
cpg	879.11	J/molxK	944.23	Joback Method
dvisc	0.0000451	Paxs	762.02	Joback Method
dvisc	0.0000607	Paxs	706.49	Joback Method

dvisc	0.0000859	Paxs	650.97	Joback Method
dvisc	0.0001296	Paxs	595.44	Joback Method
dvisc	0.0002129	Paxs	539.91	Joback Method
dvisc	0.0003918	Paxs	484.39	Joback Method
dvisc	0.0008446	Paxs	428.86	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R542119&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R542119&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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