

# Diethylmalonic acid, 2-methoxyethyl pentyl ester

Inchi:	InChI=1S/C15H28O5/c1-5-8-9-10-19-13(16)15(6-2,7-3)14(17)20-12-11-18-4/h5-12H2,1-4
InchiKey:	HSIIPTTWOLJPM-UHFFFAOYSA-N
Formula:	C15H28O5
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCCOC
Mol. weight [g/mol]:	288.38

## Physical Properties

Property code	Value	Unit	Source
gf	-494.58	kJ/mol	Joback Method
hf	-983.50	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	68.41	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.716		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	714.37	K	Joback Method
tc	896.66	K	Joback Method
tf	427.78	K	Joback Method
vc	0.930	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.91	J/molxK	714.37	Joback Method
cpg	725.12	J/molxK	744.75	Joback Method
cpg	740.47	J/molxK	775.13	Joback Method
cpg	754.97	J/molxK	805.52	Joback Method
cpg	768.62	J/molxK	835.90	Joback Method
cpg	781.44	J/molxK	866.28	Joback Method
cpg	793.43	J/molxK	896.66	Joback Method
dvisc	0.0009493	Paxs	427.78	Joback Method

dvisc	0.0004894	Paxs	475.54	Joback Method
dvisc	0.0002847	Paxs	523.31	Joback Method
dvisc	0.0001813	Paxs	571.08	Joback Method
dvisc	0.0001238	Paxs	618.84	Joback Method
dvisc	0.0000893	Paxs	666.61	Joback Method
dvisc	0.0000673	Paxs	714.37	Joback Method

## Sources

<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=U370673&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370673&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>

## 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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