

# Sebacic acid, heptyl 2-(2-methoxyethyl)heptyl ester

Inchi:	InChI=1S/C27H52O5/c1-4-6-8-13-17-22-31-26(28)19-15-11-9-10-12-16-20-27(29)32-24-
InchiKey:	KVQROMPFRMUMGR-UHFFFAOYSA-N
Formula:	C27H52O5
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)OCC(CCCCC)CCOC
Mol. weight [g/mol]:	456.70

## Physical Properties

Property code	Value	Unit	Source
gf	-398.82	kJ/mol	Joback Method
hf	-1227.71	kJ/mol	Joback Method
hfus	68.92	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.397		Crippen Method
mvol	412.040	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	991.72	K	Joback Method
tc	1229.04	K	Joback Method
tf	545.60	K	Joback Method
vc	1.607	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.72	J/molxK	991.72	Joback Method
cpg	1463.04	J/molxK	1031.27	Joback Method
cpg	1482.22	J/molxK	1070.83	Joback Method
cpg	1499.30	J/molxK	1110.38	Joback Method
cpg	1514.33	J/molxK	1149.93	Joback Method
cpg	1527.37	J/molxK	1189.49	Joback Method
cpg	1538.45	J/molxK	1229.04	Joback Method
dvisc	0.0002711	Paxs	545.60	Joback Method

dvisc	0.0001189	Paxs	619.95	Joback Method
dvisc	0.0000622	Paxs	694.31	Joback Method
dvisc	0.0000369	Paxs	768.66	Joback Method
dvisc	0.0000240	Paxs	843.01	Joback Method
dvisc	0.0000167	Paxs	917.37	Joback Method
dvisc	0.0000123	Paxs	991.72	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=U354356&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354356&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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