

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

Inchi:	InChI=1S/C26H50O5/c1-5-6-11-16-24(19-21-29-4)22-31-26(28)18-13-10-8-7-9-12-17-25
InchiKey:	SBTVYJPQFAIHKZ-UHFFFAOYSA-N
Formula:	C26H50O5
SMILES:	CCCCC(CCOC)COC(=O)CCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	442.67

## Physical Properties

Property code	Value	Unit	Source
gf	-409.68	kJ/mol	Joback Method
hf	-1212.35	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.863		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	761.84	kPa	Joback Method
rinpola	2972.00		NIST Webbook
tb	968.40	K	Joback Method
tc	1193.44	K	Joback Method
tf	519.33	K	Joback Method
vc	1.546	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.84	J/molxK	968.40	Joback Method
cpg	1461.96	J/molxK	1155.94	Joback Method
cpg	1448.82	J/molxK	1118.43	Joback Method
cpg	1433.87	J/molxK	1080.92	Joback Method
cpg	1417.09	J/molxK	1043.41	Joback Method
cpg	1398.42	J/molxK	1005.91	Joback Method
cpg	1473.33	J/molxK	1193.44	Joback Method
dvisc	0.0000132	Paxs	968.40	Joback Method
dvisc	0.0000181	Paxs	893.56	Joback Method

dvisc	0.0000264	Paxs	818.71	Joback Method
dvisc	0.0000416	Paxs	743.87	Joback Method
dvisc	0.0000725	Paxs	669.02	Joback Method
dvisc	0.0001454	Paxs	594.17	Joback Method
dvisc	0.0003561	Paxs	519.33	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=U354354&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354354&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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