

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

Inchi:	InChI=1S/C24H46O5/c1-4-6-12-15-22(18-20-27-3)21-29-24(26)17-14-11-9-8-10-13-16-2
InchiKey:	KBVYTTILAOWHEC-UHFFFAOYSA-N
Formula:	C24H46O5
SMILES:	CCCCC(CCO)COC(=O)CCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	414.62

## Physical Properties

Property code	Value	Unit	Source
gf	-424.08	kJ/mol	Joback Method
hf	-1165.79	kJ/mol	Joback Method
hfus	61.16	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	6.227		Crippen Method
mvol	369.770	ml/mol	McGowan Method
pc	845.54	kPa	Joback Method
rinpol	2803.00		NIST Webbook
rinpol	2803.00		NIST Webbook
tb	923.08	K	Joback Method
tc	1132.65	K	Joback Method
tf	511.79	K	Joback Method
vc	1.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.13	J/molxK	923.08	Joback Method
cpg	1269.91	J/molxK	958.01	Joback Method
cpg	1288.10	J/molxK	992.94	Joback Method
cpg	1304.72	J/molxK	1027.86	Joback Method
cpg	1319.81	J/molxK	1062.79	Joback Method
cpg	1333.37	J/molxK	1097.72	Joback Method
cpg	1345.43	J/molxK	1132.65	Joback Method
dvisc	0.0004053	Paxs	511.79	Joback Method

dvisc	0.0001821	Paxs	580.34	Joback Method
dvisc	0.0000969	Paxs	648.89	Joback Method
dvisc	0.0000582	Paxs	717.43	Joback Method
dvisc	0.0000382	Paxs	785.98	Joback Method
dvisc	0.0000268	Paxs	854.53	Joback Method
dvisc	0.0000198	Paxs	923.08	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354352&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354352&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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