

# Sebacic acid, butyl 5-methoxy-3-methylpentyl ester

Inchi:	InChI=1S/C21H40O5/c1-4-5-16-25-20(22)12-10-8-6-7-9-11-13-21(23)26-18-15-19(2)14-
InchiKey:	VVVRUCMJQKTYSF-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	372.54

## Physical Properties

Property code	Value	Unit	Source
gf	-449.34	kJ/mol	Joback Method
hf	-1103.87	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.056		Crippen Method
mvol	327.500	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	854.44	K	Joback Method
tc	1046.32	K	Joback Method
tf	477.98	K	Joback Method
vc	1.272	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.62	J/molxK	854.44	Joback Method
cpg	1142.77	J/molxK	1014.34	Joback Method
cpg	1129.16	J/molxK	982.36	Joback Method
cpg	1114.36	J/molxK	950.38	Joback Method
cpg	1098.34	J/molxK	918.40	Joback Method
cpg	1081.09	J/molxK	886.42	Joback Method
cpg	1155.19	J/molxK	1046.32	Joback Method
dvisc	0.0000314	Paxs	854.44	Joback Method

dvisc	0.0000422	Paxs	791.70	Joback Method
dvisc	0.0000597	Paxs	728.95	Joback Method
dvisc	0.0000901	Paxs	666.21	Joback Method
dvisc	0.0001480	Paxs	603.47	Joback Method
dvisc	0.0002731	Paxs	540.72	Joback Method
dvisc	0.0005916	Paxs	477.98	Joback Method

## Sources

<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=U355501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355501&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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