

# Sebacic acid, butyl 3-methylpentyl ester

**Inchi:** InChI=1S/C20H38O4/c1-4-6-16-23-19(21)13-11-9-7-8-10-12-14-20(22)24-17-15-18(3)5-2  
**InchiKey:** MQUNFEPWWZEBSK-UHFFFAOYSA-N  
**Formula:** C20H38O4  
**SMILES:** CCCCOC(=O)CCCCCCCC(=O)OCCC(C)CC  
**Mol. weight [g/mol]:** 342.51

## Physical Properties

Property code	Value	Unit	Source
gf	-352.76	kJ/mol	Joback Method
hf	-951.01	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.430		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	809.14	K	Joback Method
tc	993.61	K	Joback Method
tf	444.48	K	Joback Method
vc	1.198	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.66	J/molxK	809.14	Joback Method
cpg	987.99	J/molxK	839.88	Joback Method
cpg	1005.26	J/molxK	870.63	Joback Method
cpg	1021.49	J/molxK	901.37	Joback Method
cpg	1036.69	J/molxK	932.12	Joback Method
cpg	1050.89	J/molxK	962.86	Joback Method
cpg	1064.10	J/molxK	993.61	Joback Method
dvisc	0.0009916	Paxs	444.48	Joback Method

dvisc	0.0004441	Paxs	505.26	Joback Method
dvisc	0.0002364	Paxs	566.03	Joback Method
dvisc	0.0001422	Paxs	626.81	Joback Method
dvisc	0.0000935	Paxs	687.59	Joback Method
dvisc	0.0000659	Paxs	748.36	Joback Method
dvisc	0.0000489	Paxs	809.14	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=U355615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355615&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>

## 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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