

# Sebacic acid, butyl pent-4-enyl ester

<b>Inchi:</b>	InChI=1S/C19H34O4/c1-3-5-13-17-23-19(21)15-12-10-8-7-9-11-14-18(20)22-16-6-4-2/h3
<b>InchiKey:</b>	HAVLQGQUEFAVFN-UHFFFAOYSA-N
<b>Formula:</b>	C19H34O4
<b>SMILES:</b>	C=CCCCOC(=O)CCCCCCCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	326.47

## Physical Properties

Property code	Value	Unit	Source
gf	-270.90	kJ/mol	Joback Method
hf	-799.66	kJ/mol	Joback Method
hfus	49.26	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.960		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	783.38	K	Joback Method
tc	964.87	K	Joback Method
tf	446.45	K	Joback Method
vc	1.129	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.52	J/molxK	783.38	Joback Method
cpg	899.80	J/molxK	813.63	Joback Method
cpg	916.15	J/molxK	843.88	Joback Method
cpg	931.56	J/molxK	874.12	Joback Method
cpg	946.06	J/molxK	904.37	Joback Method
cpg	959.66	J/molxK	934.62	Joback Method
cpg	972.38	J/molxK	964.87	Joback Method
dvisc	0.0009442	Paxs	446.45	Joback Method

dvisc	0.0004720	Paxs	502.61	Joback Method
dvisc	0.0002712	Paxs	558.76	Joback Method
dvisc	0.0001724	Paxs	614.92	Joback Method
dvisc	0.0001183	Paxs	671.07	Joback Method
dvisc	0.0000860	Paxs	727.23	Joback Method
dvisc	0.0000654	Paxs	783.38	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=U355411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355411&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>

## 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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