

# Sebacic acid, isobutyl 3-methylbut-2-enyl ester

<b>Inchi:</b>	InChI=1S/C19H34O4/c1-16(2)13-14-22-18(20)11-9-7-5-6-8-10-12-19(21)23-15-17(3)4/h1
<b>InchiKey:</b>	UMPSXCBTIVYCMC-UHFFFAOYSA-N
<b>Formula:</b>	C19H34O4
<b>SMILES:</b>	CC(C)=CCOC(=O)CCCCCCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	326.47

## Physical Properties

Property code	Value	Unit	Source
gf	-289.51	kJ/mol	Joback Method
hf	-822.94	kJ/mol	Joback Method
hfus	45.91	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.816		Crippen Method
mvol	289.150	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	2260.00		NIST Webbook
tb	790.30	K	Joback Method
tc	976.49	K	Joback Method
tf	414.17	K	Joback Method
vc	1.123	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.21	J/mol×K	790.30	Joback Method
cpg	901.71	J/mol×K	821.33	Joback Method
cpg	918.23	J/mol×K	852.36	Joback Method
cpg	933.81	J/mol×K	883.40	Joback Method
cpg	948.46	J/mol×K	914.43	Joback Method
cpg	962.21	J/mol×K	945.46	Joback Method
cpg	975.09	J/mol×K	976.49	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=U355876&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355876&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>cpg:</b>	Ideal gas heat capacity
<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>hvac:</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>mccol:</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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