

# Sebacic acid, isobutyl 4-methylpent-2-yl ester

<b>Inchi:</b>	InChI=1S/C20H38O4/c1-16(2)14-18(5)24-20(22)13-11-9-7-6-8-10-12-19(21)23-15-17(3)
<b>InchiKey:</b>	FZELVCLPTDINCY-UHFFFAOYSA-N
<b>Formula:</b>	C20H38O4
<b>SMILES:</b>	CC(C)COC(=O)CCCCCCCCC(=O)OC(C)CC(C)C
<b>Mol. weight [g/mol]:</b>	342.51

## Physical Properties

Property code	Value	Unit	Source
gf	-357.64	kJ/mol	Joback Method
hf	-961.57	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	77.26	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.284		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	2209.00		NIST Webbook
rinpol	2209.00		NIST Webbook
tb	808.26	K	Joback Method
tc	994.56	K	Joback Method
tf	414.48	K	Joback Method
vc	1.185	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.62	J/molxK	808.26	Joback Method
cpg	989.13	J/molxK	839.31	Joback Method
cpg	1006.54	J/molxK	870.36	Joback Method
cpg	1022.88	J/molxK	901.41	Joback Method
cpg	1038.15	J/molxK	932.46	Joback Method
cpg	1052.38	J/molxK	963.51	Joback Method
cpg	1065.59	J/molxK	994.56	Joback Method
dvisc	0.0014761	Paxs	414.48	Joback Method

dvisc	0.0005410	Paxs	480.11	Joback Method
dvisc	0.0002524	Paxs	545.74	Joback Method
dvisc	0.0001387	Paxs	611.37	Joback Method
dvisc	0.0000856	Paxs	677.00	Joback Method
dvisc	0.0000575	Paxs	742.63	Joback Method
dvisc	0.0000412	Paxs	808.26	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355349&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355349&amp;Units=SI</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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