

# Sebacic acid, isobutyl 4-methylhept-3-yl ester

**Inchi:** InChI=1S/C22H42O4/c1-6-14-19(5)20(7-2)26-22(24)16-13-11-9-8-10-12-15-21(23)25-17  
**InchiKey:** QPWKPGOSDDTMIK-UHFFFAOYSA-N  
**Formula:** C22H42O4  
**SMILES:** CCCC(C)C(CC)OC(=O)CCCCCCCC(=O)OCC(C)C  
**Mol. weight [g/mol]:** 370.57

## Physical Properties

Property code	Value	Unit	Source
gf	-340.80	kJ/mol	Joback Method
hf	-1002.85	kJ/mol	Joback Method
hfus	47.74	kJ/mol	Joback Method
hvap	81.71	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.064		Crippen Method
mvol	335.720	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	1912.00		NIST Webbook
tb	854.02	K	Joback Method
tc	1046.45	K	Joback Method
tf	437.02	K	Joback Method
vc	1.298	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.43	J/molxK	854.02	Joback Method
cpg	1177.30	J/molxK	1014.38	Joback Method
cpg	1162.90	J/molxK	982.31	Joback Method
cpg	1147.34	J/molxK	950.24	Joback Method
cpg	1130.59	J/molxK	918.16	Joback Method
cpg	1112.63	J/molxK	886.09	Joback Method
cpg	1190.56	J/molxK	1046.45	Joback Method
dvisc	0.0000305	Paxs	854.02	Joback Method
dvisc	0.0000427	Paxs	784.52	Joback Method

dvisc	0.0000637	Paxs	715.02	Joback Method
dvisc	0.0001037	Paxs	645.52	Joback Method
dvisc	0.0001897	Paxs	576.02	Joback Method
dvisc	0.0004097	Paxs	506.52	Joback Method
dvisc	0.0011301	Paxs	437.02	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416197&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416197&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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

Latest version available from:

<https://www.chemeo.com/cid/95-881-9/Sebacic-acid-isobutyl-4-methylhept-3-yl-ester.pdf>

Generated by Cheméo on 2024-04-25 08:09:53.062780027 +0000 UTC m=+16321841.983357369.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.