

# Sebacic acid, heptyl propyl ester

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

## Physical Properties

Property code	Value	Unit	Source
gf	-350.32	kJ/mol	Joback Method
hf	-945.73	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.574		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1077.81	kPa	Joback Method
rinsol	2424.00		NIST Webbook
tb	809.58	K	Joback Method
tc	993.33	K	Joback Method
tf	459.48	K	Joback Method
vc	1.204	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.18	J/molxK	809.58	Joback Method
cpg	987.44	J/molxK	840.20	Joback Method
cpg	1004.65	J/molxK	870.83	Joback Method
cpg	1020.84	J/molxK	901.45	Joback Method
cpg	1036.02	J/molxK	932.08	Joback Method
cpg	1050.21	J/molxK	962.70	Joback Method
cpg	1063.43	J/molxK	993.33	Joback Method
dvisc	0.0008397	Paxs	459.48	Joback Method
dvisc	0.0004093	Paxs	517.83	Joback Method

dvisc	0.0002308	Paxs	576.18	Joback Method
dvisc	0.0001446	Paxs	634.53	Joback Method
dvisc	0.0000980	Paxs	692.88	Joback Method
dvisc	0.0000706	Paxs	751.23	Joback Method
dvisc	0.0000533	Paxs	809.58	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=U354304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354304&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

Latest version available from:

<https://www.chemeo.com/cid/17-029-1/Sebacic-acid-heptyl-propyl-ester.pdf>

Generated by Cheméo on 2024-04-28 21:57:35.238949295 +0000 UTC m=+16630704.159526610.

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