

# Sebacic acid, di(2-propylpentyl) ester

<b>Inchi:</b>	InChI=1S/C26H50O4/c1-5-15-23(16-6-2)21-29-25(27)19-13-11-9-10-12-14-20-26(28)30-
<b>InchiKey:</b>	ZMNXATLFJJQIPI-UHFFFAOYSA-N
<b>Formula:</b>	C26H50O4
<b>SMILES:</b>	CCCC(CCC)COC(=O)CCCCCCCCC(=O)OCC(CCC)CCC
<b>Mol. weight [g/mol]:</b>	426.67

## Physical Properties

Property code	Value	Unit	Source
gf	-304.68	kJ/mol	Joback Method
hf	-1080.13	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.626		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	945.98	K	Joback Method
tc	1162.69	K	Joback Method
tf	497.10	K	Joback Method
vc	1.528	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.96	J/molxK	945.98	Joback Method
cpg	1435.00	J/molxK	1126.57	Joback Method
cpg	1420.33	J/molxK	1090.45	Joback Method
cpg	1404.14	J/molxK	1054.33	Joback Method
cpg	1386.38	J/molxK	1018.22	Joback Method
cpg	1367.00	J/molxK	982.10	Joback Method
cpg	1448.19	J/molxK	1162.69	Joback Method
dvisc	0.0000180	Paxs	945.98	Joback Method

dvisc	0.0000248	Paxs	871.17	Joback Method
dvisc	0.0000365	Paxs	796.35	Joback Method
dvisc	0.0000581	Paxs	721.54	Joback Method
dvisc	0.0001030	Paxs	646.73	Joback Method
dvisc	0.0002121	Paxs	571.91	Joback Method
dvisc	0.0005428	Paxs	497.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416221&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416221&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>mccvol:</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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