

# Sebacic acid, 3,4-dimethylphenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C24H38O4/c1-4-5-6-13-18-27-23(25)14-11-9-7-8-10-12-15-24(26)28-22-17-16
<b>InchiKey:</b>	SOKAOXDRCZKKJD-UHFFFAOYSA-N
<b>Formula:</b>	C24H38O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(C)c(C)c1
<b>Mol. weight [g/mol]:</b>	390.56

## Physical Properties

Property code	Value	Unit	Source
gf	-223.49	kJ/mol	Joback Method
hf	-814.70	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.453		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	3011.00		NIST Webbook
rinpol	3011.00		NIST Webbook
tb	937.74	K	Joback Method
tc	1148.48	K	Joback Method
tf	556.02	K	Joback Method
vc	1.319	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.89	J/molxK	937.74	Joback Method
cpg	1135.82	J/molxK	972.86	Joback Method
cpg	1151.36	J/molxK	1007.99	Joback Method
cpg	1165.54	J/molxK	1043.11	Joback Method
cpg	1178.40	J/molxK	1078.24	Joback Method
cpg	1189.97	J/molxK	1113.36	Joback Method
cpg	1200.28	J/molxK	1148.48	Joback Method
dvisc	0.0003364	Paxs	556.02	Joback Method

dvisc	0.0001850	Paxs	619.64	Joback Method
dvisc	0.0001137	Paxs	683.26	Joback Method
dvisc	0.0000760	Paxs	746.88	Joback Method
dvisc	0.0000540	Paxs	810.50	Joback Method
dvisc	0.0000404	Paxs	874.12	Joback Method
dvisc	0.0000314	Paxs	937.74	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=U354582&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354582&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> 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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