

# Sebacic acid, 2,3-dimethylphenyl octyl ester

<b>Inchi:</b>	InChI=1S/C26H42O4/c1-4-5-6-7-12-15-21-29-25(27)19-13-10-8-9-11-14-20-26(28)30-24
<b>InchiKey:</b>	MWCMIKVPEBWRHR-UHFFFAOYSA-N
<b>Formula:</b>	C26H42O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1C
<b>Mol. weight [g/mol]:</b>	418.61

## Physical Properties

Property code	Value	Unit	Source
gf	-206.65	kJ/mol	Joback Method
hf	-855.98	kJ/mol	Joback Method
hfus	61.93	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.233		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	3143.00		NIST Webbook
tb	983.50	K	Joback Method
tc	1204.69	K	Joback Method
tf	578.56	K	Joback Method
vc	1.431	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.12	J/molxK	983.50	Joback Method
cpg	1260.57	J/molxK	1020.37	Joback Method
cpg	1276.44	J/molxK	1057.23	Joback Method
cpg	1290.78	J/molxK	1094.10	Joback Method
cpg	1303.62	J/molxK	1130.96	Joback Method
cpg	1315.02	J/molxK	1167.83	Joback Method
cpg	1325.02	J/molxK	1204.69	Joback Method
dvisc	0.0002672	Paxs	578.56	Joback Method
dvisc	0.0001440	Paxs	646.05	Joback Method

dvisc	0.0000872	Paxs	713.54	Joback Method
dvisc	0.0000576	Paxs	781.03	Joback Method
dvisc	0.0000406	Paxs	848.52	Joback Method
dvisc	0.0000302	Paxs	916.01	Joback Method
dvisc	0.0000233	Paxs	983.50	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=U355211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355211&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

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