

# Sebacic acid, 4-methylbenzyl octyl ester

<b>Inchi:</b>	InChI=1S/C26H42O4/c1-3-4-5-6-11-14-21-29-25(27)15-12-9-7-8-10-13-16-26(28)30-22-2
<b>InchiKey:</b>	RTRZKNZLYNGFSK-UHFFFAOYSA-N
<b>Formula:</b>	C26H42O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCCCCC(=O)OCc1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	418.61

## Physical Properties

Property code	Value	Unit	Source
gf	-197.02	kJ/mol	Joback Method
hf	-844.51	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.063		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
tb	978.52	K	Joback Method
tc	1198.52	K	Joback Method
tf	566.04	K	Joback Method
vc	1.431	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.68	J/molxK	978.52	Joback Method
cpg	1316.64	J/molxK	1161.85	Joback Method
cpg	1304.93	J/molxK	1125.19	Joback Method
cpg	1291.83	J/molxK	1088.52	Joback Method
cpg	1277.29	J/molxK	1051.85	Joback Method
cpg	1261.26	J/molxK	1015.19	Joback Method
cpg	1327.00	J/molxK	1198.52	Joback Method
dvisc	0.0000228	Paxs	978.52	Joback Method

dvisc	0.0000298	Paxs	909.77	Joback Method
dvisc	0.0000407	Paxs	841.03	Joback Method
dvisc	0.0000589	Paxs	772.28	Joback Method
dvisc	0.0000914	Paxs	703.53	Joback Method
dvisc	0.0001561	Paxs	634.79	Joback Method
dvisc	0.0003036	Paxs	566.04	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=U380708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380708&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>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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