

# Sebacic acid, 2,3-dimethylphenyl pentyl ester

<b>Inchi:</b>	InChI=1S/C23H36O4/c1-4-5-12-18-26-22(24)16-10-8-6-7-9-11-17-23(25)27-21-15-13-14
<b>InchiKey:</b>	MNCVVIPXQFMQCG-UHFFFAOYSA-N
<b>Formula:</b>	C23H36O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1C
<b>Mol. weight [g/mol]:</b>	376.53

## Physical Properties

Property code	Value	Unit	Source
gf	-231.91	kJ/mol	Joback Method
hf	-794.06	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.063		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinqol	2835.00		NIST Webbook
tb	914.86	K	Joback Method
tc	1121.86	K	Joback Method
tf	544.75	K	Joback Method
vc	1.264	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.52	J/molxK	914.86	Joback Method
cpg	1128.16	J/molxK	1087.36	Joback Method
cpg	1116.54	J/molxK	1052.86	Joback Method
cpg	1103.70	J/molxK	1018.36	Joback Method
cpg	1089.60	J/molxK	983.86	Joback Method
cpg	1074.21	J/molxK	949.36	Joback Method
cpg	1138.58	J/molxK	1121.86	Joback Method
dvisc	0.0000364	Paxs	914.86	Joback Method
dvisc	0.0000466	Paxs	853.17	Joback Method

dvisc	0.0000621	Paxs	791.49	Joback Method
dvisc	0.0000869	Paxs	729.80	Joback Method
dvisc	0.0001294	Paxs	668.12	Joback Method
dvisc	0.0002088	Paxs	606.43	Joback Method
dvisc	0.0003755	Paxs	544.75	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=U355207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355207&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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