

# Sebacic acid, 2,5-dimethylphenyl dodecyl ester

Inchi:	InChI=1S/C30H50O4/c1-4-5-6-7-8-9-10-13-16-19-24-33-29(31)20-17-14-11-12-15-18-21
InchiKey:	MVQSVTRVDIDLLI-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)ccc1C
Mol. weight [g/mol]:	474.72

## Physical Properties

Property code	Value	Unit	Source
gf	-172.97	kJ/mol	Joback Method
hf	-938.54	kJ/mol	Joback Method
hfus	72.29	kJ/mol	Joback Method
hvap	104.29	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	8.794		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	728.49	kPa	Joback Method
rinpola	3503.00		NIST Webbook
tb	1075.02	K	Joback Method
tc	1331.15	K	Joback Method
tf	623.64	K	Joback Method
vc	1.655	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.08	J/molxK	1075.02	Joback Method
cpg	1514.89	J/molxK	1117.71	Joback Method
cpg	1531.53	J/molxK	1160.40	Joback Method
cpg	1546.08	J/molxK	1203.08	Joback Method
cpg	1558.64	J/molxK	1245.77	Joback Method
cpg	1569.31	J/molxK	1288.46	Joback Method
cpg	1578.16	J/molxK	1331.15	Joback Method
dvisc	0.0001630	Paxs	623.64	Joback Method
dvisc	0.0000846	Paxs	698.87	Joback Method

dvisc	0.0000498	Paxs	774.10	Joback Method
dvisc	0.0000323	Paxs	849.33	Joback Method
dvisc	0.0000224	Paxs	924.56	Joback Method
dvisc	0.0000164	Paxs	999.79	Joback Method
dvisc	0.0000126	Paxs	1075.02	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=U354983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354983&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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