

# Sebacic acid, dodecyl 3-methylbut-3-enyl ester

<b>Inchi:</b>	InChI=1S/C27H50O4/c1-4-5-6-7-8-9-10-13-16-19-23-30-26(28)20-17-14-11-12-15-18-21
<b>InchiKey:</b>	DIDHUAXJKCUHCQ-UHFFFAOYSA-N
<b>Formula:</b>	C27H50O4
<b>SMILES:</b>	<chem>C=C(C)CCOC(=O)CCCCCCCC(=O)OCCCCCCCCCCC</chem>
<b>Mol. weight [g/mol]:</b>	438.68

## Physical Properties

Property code	Value	Unit	Source
gf	-212.09	kJ/mol	Joback Method
hf	-974.57	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mvol	401.870	ml/mol	McGowan Method
pc	742.05	kPa	Joback Method
rinpol	3058.00		NIST Webbook
rinpol	3058.00		NIST Webbook
tb	966.30	K	Joback Method
tc	1191.27	K	Joback Method
tf	522.65	K	Joback Method
vc	1.577	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.32	J/molxK	966.30	Joback Method
cpg	1400.62	J/molxK	1003.79	Joback Method
cpg	1420.22	J/molxK	1041.29	Joback Method
cpg	1438.18	J/molxK	1078.78	Joback Method
cpg	1454.57	J/molxK	1116.28	Joback Method
cpg	1469.46	J/molxK	1153.77	Joback Method
cpg	1482.91	J/molxK	1191.27	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=U355943&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355943&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>h vap:</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>r in pol:</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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