

# Sebacic acid, dodec-9-ynyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C26H46O4/c1-4-5-6-7-8-9-10-13-16-19-22-29-25(27)20-17-14-11-12-15-18-21
<b>InchiKey:</b>	DPODJGITTSGQMV-UHFFFAOYSA-N
<b>Formula:</b>	C26H46O4
<b>SMILES:</b>	CCC#CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	422.64

## Physical Properties

Property code	Value	Unit	Source
gf	-99.44	kJ/mol	Joback Method
hf	-802.55	kJ/mol	Joback Method
hfus	68.27	kJ/mol	Joback Method
hvap	93.55	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	6.994		Crippen Method
mvol	383.480	ml/mol	McGowan Method
pc	838.21	kPa	Joback Method
rmpol	2983.00		NIST Webbook
tb	955.42	K	Joback Method
tc	1170.99	K	Joback Method
tf	618.20	K	Joback Method
vc	1.496	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.21	J/molxK	955.42	Joback Method
cpg	1310.69	J/molxK	991.35	Joback Method
cpg	1328.62	J/molxK	1027.28	Joback Method
cpg	1345.05	J/molxK	1063.21	Joback Method
cpg	1360.01	J/molxK	1099.13	Joback Method
cpg	1373.54	J/molxK	1135.06	Joback Method
cpg	1385.70	J/molxK	1170.99	Joback Method

# Sources

<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>
<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=U355789&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355789&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>

# 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>hvac:</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>mccol:</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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