

# Sebacic acid, butyl dodec-9-ynyl ester

<b>Inchi:</b>	InChI=1S/C26H46O4/c1-3-5-7-8-9-10-11-14-17-20-24-30-26(28)22-19-16-13-12-15-18-2
<b>InchiKey:</b>	WCIWBTIIJQRGGC-UHFFFAOYSA-N
<b>Formula:</b>	C26H46O4
<b>SMILES:</b>	CCC#CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	422.64

## Physical Properties

Property code	Value	Unit	Source
gf	-97.00	kJ/mol	Joback Method
hf	-797.27	kJ/mol	Joback Method
hfus	71.79	kJ/mol	Joback Method
hvap	93.93	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.138		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	834.35	kPa	Joback Method
rinsol	3027.00		NIST Webbook
tb	955.86	K	Joback Method
tc	1172.24	K	Joback Method
tf	633.20	K	Joback Method
vc	1.502	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.85	J/molxK	955.86	Joback Method
cpg	1310.44	J/molxK	991.92	Joback Method
cpg	1328.48	J/molxK	1027.99	Joback Method
cpg	1345.02	J/molxK	1064.05	Joback Method
cpg	1360.10	J/molxK	1100.11	Joback Method
cpg	1373.76	J/molxK	1136.17	Joback Method
cpg	1386.04	J/molxK	1172.24	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355790&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355790&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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>rinpola:</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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