

# Sebacic acid, but-3-yn-2-yl octyl ester

<b>Inchi:</b>	InChI=1S/C22H38O4/c1-4-6-7-8-13-16-19-25-21(23)17-14-11-9-10-12-15-18-22(24)26-2
<b>InchiKey:</b>	CVJWVMVFLQGXEN-UHFFFAOYSA-N
<b>Formula:</b>	C22H38O4
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCCCCCC</chem>
<b>Mol. weight [g/mol]:</b>	366.53

## Physical Properties

Property code	Value	Unit	Source
gf	-112.85	kJ/mol	Joback Method
hf	-700.39	kJ/mol	Joback Method
hfus	57.76	kJ/mol	Joback Method
hvap	82.35	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.576		Crippen Method
mvol	327.120	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2489.00		NIST Webbook
tb	845.02	K	Joback Method
tc	1036.58	K	Joback Method
tf	513.99	K	Joback Method
vc	1.272	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.77	J/mol×K	845.02	Joback Method
cpg	1052.81	J/mol×K	876.95	Joback Method
cpg	1069.74	J/mol×K	908.87	Joback Method
cpg	1085.59	J/mol×K	940.80	Joback Method
cpg	1100.39	J/mol×K	972.73	Joback Method
cpg	1114.17	J/mol×K	1004.66	Joback Method
cpg	1126.96	J/mol×K	1036.58	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=U355850&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355850&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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