

# Sebacic acid, ethyl 1-phenylpropyl ester

<b>Inchi:</b>	InChI=1S/C21H32O4/c1-3-19(18-14-10-9-11-15-18)25-21(23)17-13-8-6-5-7-12-16-20(22)
<b>InchiKey:</b>	JIWNPKVYLBGDU-UHFFFAOYSA-N
<b>Formula:</b>	C21H32O4
<b>SMILES:</b>	CCOC(=O)CCCCCCCC(=O)OC(CC)c1ccccc1
<b>Mol. weight [g/mol]:</b>	348.48

## Physical Properties

Property code	Value	Unit	Source
gf	-231.93	kJ/mol	Joback Method
hf	-735.12	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.365		Crippen Method
mvol	297.870	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	2472.00		NIST Webbook
tb	858.70	K	Joback Method
tc	1060.45	K	Joback Method
tf	482.17	K	Joback Method
vc	1.145	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.24	J/molxK	858.70	Joback Method
cpg	954.76	J/molxK	892.33	Joback Method
cpg	970.10	J/molxK	925.95	Joback Method
cpg	984.26	J/molxK	959.58	Joback Method
cpg	997.29	J/molxK	993.20	Joback Method
cpg	1009.22	J/molxK	1026.83	Joback Method
cpg	1020.07	J/molxK	1060.45	Joback Method
dvisc	0.0007178	Paxs	482.17	Joback Method
dvisc	0.0003427	Paxs	544.92	Joback Method

dvisc	0.0001906	Paxs	607.68	Joback Method
dvisc	0.0001183	Paxs	670.43	Joback Method
dvisc	0.0000797	Paxs	733.19	Joback Method
dvisc	0.0000571	Paxs	795.94	Joback Method
dvisc	0.0000430	Paxs	858.70	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=U354985&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354985&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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