

# Sebacic acid, butyl 2-phenoxyethyl ester

<b>Inchi:</b>	InChI=1S/C22H34O5/c1-2-3-17-26-21(23)15-11-6-4-5-7-12-16-22(24)27-19-18-25-20-13
<b>InchiKey:</b>	OMIDJFJLDYOFOZ-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O5
<b>SMILES:</b>	CCCCOC(=O)CCCCCCCC(=O)OCCOc1ccccc1
<b>Mol. weight [g/mol]:</b>	378.50

## Physical Properties

Property code	Value	Unit	Source
gf	-326.07	kJ/mol	Joback Method
hf	-882.70	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	87.56	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.073		Crippen Method
mvol	317.830	ml/mol	McGowan Method
pc	1169.62	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	904.44	K	Joback Method
tc	1109.57	K	Joback Method
tf	530.67	K	Joback Method
vc	1.226	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.65	J/molxK	904.44	Joback Method
cpg	1095.08	J/molxK	1075.38	Joback Method
cpg	1084.17	J/molxK	1041.19	Joback Method
cpg	1072.00	J/molxK	1007.01	Joback Method
cpg	1058.53	J/molxK	972.82	Joback Method
cpg	1043.76	J/molxK	938.63	Joback Method
cpg	1104.75	J/molxK	1109.57	Joback Method
dvisc	0.0000302	Paxs	904.44	Joback Method

dvisc	0.0000395	Paxs	842.14	Joback Method
dvisc	0.0000538	Paxs	779.85	Joback Method
dvisc	0.0000775	Paxs	717.55	Joback Method
dvisc	0.0001196	Paxs	655.26	Joback Method
dvisc	0.0002022	Paxs	592.96	Joback Method
dvisc	0.0003866	Paxs	530.67	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380782&amp;Units=SI</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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