

# Succinic acid, heptyl 2-phenoxyethyl ester

<b>Inchi:</b>	InChI=1S/C19H28O5/c1-2-3-4-5-9-14-23-18(20)12-13-19(21)24-16-15-22-17-10-7-6-8-1
<b>InchiKey:</b>	KOEAGLHVTQCAIL-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O5
<b>SMILES:</b>	CCCCCCCOC(=O)CCC(=O)OCCOc1ccccc1
<b>Mol. weight [g/mol]:</b>	336.42

## Physical Properties

Property code	Value	Unit	Source
gf	-351.33	kJ/mol	Joback Method
hf	-820.78	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	80.89	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.902		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinsol	2459.00		NIST Webbook
tb	835.80	K	Joback Method
tc	1035.35	K	Joback Method
tf	496.86	K	Joback Method
vc	1.058	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.89	J/molxK	835.80	Joback Method
cpg	864.43	J/molxK	869.06	Joback Method
cpg	878.82	J/molxK	902.32	Joback Method
cpg	892.08	J/molxK	935.58	Joback Method
cpg	904.21	J/molxK	968.84	Joback Method
cpg	915.23	J/molxK	1002.09	Joback Method
cpg	925.15	J/molxK	1035.35	Joback Method
dvisc	0.0005380	Paxs	496.86	Joback Method
dvisc	0.0002909	Paxs	553.35	Joback Method

dvisc	0.0001763	Paxs	609.84	Joback Method
dvisc	0.0001163	Paxs	666.33	Joback Method
dvisc	0.0000819	Paxs	722.82	Joback Method
dvisc	0.0000607	Paxs	779.31	Joback Method
dvisc	0.0000468	Paxs	835.80	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=U381198&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381198&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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