

# Succinic acid, hex-4-yn-3-yl 1-phenylpropyl ester

Inchi:	InChI=1S/C19H24O4/c1-4-10-16(5-2)22-18(20)13-14-19(21)23-17(6-3)15-11-8-7-9-12-15
InchiKey:	NRJSAWAWRSPXOV-UHFFFAOYSA-N
Formula:	C19H24O4
SMILES:	CC#CC(CC)OC(=O)CCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]:	316.39

## Physical Properties

Property code	Value	Unit	Source
gf	-48.41	kJ/mol	Joback Method
hf	-426.82	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.806		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
tb	821.50	K	Joback Method
tc	1039.52	K	Joback Method
tf	550.73	K	Joback Method
vc	0.990	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.25	J/molxK	821.50	Joback Method
cpg	785.98	J/molxK	857.84	Joback Method
cpg	800.49	J/molxK	894.17	Joback Method
cpg	813.80	J/molxK	930.51	Joback Method
cpg	825.94	J/molxK	966.85	Joback Method
cpg	836.94	J/molxK	1003.18	Joback Method
cpg	846.83	J/molxK	1039.52	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=U389927&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389927&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>
<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>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>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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