

# Succinic acid, tridec-2-yn-1-yl 1-phenylpropyl ester

Inchi:	InChI=1S/C26H38O4/c1-3-5-6-7-8-9-10-11-12-13-17-22-29-25(27)20-21-26(28)30-24(4-2
InchiKey:	BDEYEIUWEBAEBW-UHFFFAOYSA-N
Formula:	C26H38O4
SMILES:	CCCCCCCCC#CCOC(=O)CCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]:	414.58

## Physical Properties

Property code	Value	Unit	Source
gf	12.97	kJ/mol	Joback Method
hf	-566.02	kJ/mol	Joback Method
hfus	62.31	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.538		Crippen Method
mvol	359.720	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	982.10	K	Joback Method
tc	1203.17	K	Joback Method
tf	644.62	K	Joback Method
vc	1.387	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.48	J/mol×K	982.10	Joback Method
cpg	1204.86	J/mol×K	1018.94	Joback Method
cpg	1219.78	J/mol×K	1055.79	Joback Method
cpg	1233.28	J/mol×K	1092.63	Joback Method
cpg	1245.43	J/mol×K	1129.48	Joback Method
cpg	1256.26	J/mol×K	1166.32	Joback Method
cpg	1265.84	J/mol×K	1203.17	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=U389937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389937&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>h vap:</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>r in pol:</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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