

# Succinic acid, 4-cyanophenyl 3,4-dimethylphenyl ester

**Inchi:** InChI=1S/C19H17NO4/c1-13-3-6-17(11-14(13)2)24-19(22)10-9-18(21)23-16-7-4-15(12-2)  
**InchiKey:** YJADWINZDREEFX-UHFFFAOYSA-N  
**Formula:** C19H17NO4  
**SMILES:** Cc1ccc(OC(=O)CCC(=O)Oc2ccc(C#N)cc2)cc1C  
**Mol. weight [g/mol]:** 323.34

## Physical Properties

Property code	Value	Unit	Source
gf	-29.63	kJ/mol	Joback Method
hf	-321.56	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	93.22	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.466		Crippen Method
mcvol	247.310	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	957.08	K	Joback Method
tc	1195.87	K	Joback Method
tf	603.60	K	Joback Method
vc	0.958	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.05	J/molxK	957.08	Joback Method
cpg	744.16	J/molxK	996.88	Joback Method
cpg	752.98	J/molxK	1036.68	Joback Method
cpg	760.53	J/molxK	1076.48	Joback Method
cpg	766.81	J/molxK	1116.27	Joback Method
cpg	771.87	J/molxK	1156.07	Joback Method
cpg	775.72	J/molxK	1195.87	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=U360707&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360707&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpola:</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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