

# Succinic acid, ethyl 2-tertbutyl-6-methylphenyl ester

Inchi:	InChI=1S/C17H24O4/c1-6-20-14(18)10-11-15(19)21-16-12(2)8-7-9-13(16)17(3,4)5/h7-9H
InchiKey:	VWVUCNYMGRFTJX-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CCOC(=O)CCC(=O)Oc1c(C)cccc1C(C)(C)C
Mol. weight [g/mol]:	292.37

## Physical Properties

Property code	Value	Unit	Source
gf	-279.59	kJ/mol	Joback Method
hf	-678.97	kJ/mol	Joback Method
hfus	31.21	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.541		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	774.35	K	Joback Method
tc	983.43	K	Joback Method
tf	479.55	K	Joback Method
vc	0.916	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.40	J/molxK	774.35	Joback Method
cpg	773.05	J/molxK	948.59	Joback Method
cpg	761.55	J/molxK	913.74	Joback Method
cpg	749.06	J/molxK	878.89	Joback Method
cpg	735.56	J/molxK	844.04	Joback Method
cpg	721.02	J/molxK	809.20	Joback Method
cpg	783.59	J/molxK	983.43	Joback Method
dvisc	0.0000670	Paxs	774.35	Joback Method

dvisc	0.0000858	Paxs	725.22	Joback Method
dvisc	0.0001138	Paxs	676.08	Joback Method
dvisc	0.0001578	Paxs	626.95	Joback Method
dvisc	0.0002313	Paxs	577.82	Joback Method
dvisc	0.0003639	Paxs	528.68	Joback Method
dvisc	0.0006285	Paxs	479.55	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=U349635&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349635&amp;Units=SI</a>
<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>

## 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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