

# Succinic acid, 3-methylbut-2-en-1-yl 3-ethylphenyl ester

Inchi:	InChI=1S/C17H22O4/c1-4-14-6-5-7-15(12-14)21-17(19)9-8-16(18)20-11-10-13(2)3/h5-7,
InchiKey:	XBCFJHBEZARQDN-UHFFFAOYSA-N
Formula:	C17H22O4
SMILES:	CCc1cccc(OC(=O)CCC(=O)OCC=C(C)C)c1
Mol. weight [g/mol]:	290.35

## Physical Properties

Property code	Value	Unit	Source
gf	-201.13	kJ/mol	Joback Method
hf	-551.32	kJ/mol	Joback Method
hfus	37.90	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.444		Crippen Method
mvol	237.210	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	776.64	K	Joback Method
tc	985.28	K	Joback Method
tf	445.57	K	Joback Method
vc	0.908	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.98	J/molxK	776.64	Joback Method
cpg	694.05	J/molxK	811.41	Joback Method
cpg	708.12	J/molxK	846.19	Joback Method
cpg	721.21	J/molxK	880.96	Joback Method
cpg	733.34	J/molxK	915.73	Joback Method
cpg	744.56	J/molxK	950.50	Joback Method
cpg	754.88	J/molxK	985.28	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=U390099&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390099&amp;Units=SI</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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