

# Succinic acid, 1,1,1-trifluoroprop-2-yl 3-ethylphenyl ester

<b>Inchi:</b>	InChI=1S/C15H17F3O4/c1-3-11-5-4-6-12(9-11)22-14(20)8-7-13(19)21-10(2)15(16,17)18
<b>InchiKey:</b>	LYSWHIQMQJLLSJ-UHFFFAOYSA-N
<b>Formula:</b>	C15H17F3O4
<b>SMILES:</b>	CCc1cccc(OC(=O)CCC(=O)OC(C)C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	318.29

## Physical Properties

Property code	Value	Unit	Source
gf	-873.67	kJ/mol	Joback Method
hf	-1219.83	kJ/mol	Joback Method
hfus	32.13	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.429		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1722.00		NIST Webbook
rinpol	1722.00		NIST Webbook
tb	720.98	K	Joback Method
tc	915.14	K	Joback Method
tf	431.26	K	Joback Method
vc	0.853	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.09	J/mol×K	720.98	Joback Method
cpg	633.73	J/mol×K	753.34	Joback Method
cpg	646.46	J/mol×K	785.70	Joback Method
cpg	658.31	J/mol×K	818.06	Joback Method
cpg	669.32	J/mol×K	850.42	Joback Method
cpg	679.50	J/mol×K	882.78	Joback Method
cpg	688.88	J/mol×K	915.14	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=U390093&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390093&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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