

# Succinic acid, ethyl 4-trifluoromethoxybenzyl ester

Inchi:	InChI=1S/C14H15F3O5/c1-2-20-12(18)7-8-13(19)21-9-10-3-5-11(6-4-10)22-14(15,16)17
InchiKey:	KKEJXQUCMJRKBV-UHFFFAOYSA-N
Formula:	C14H15F3O5
SMILES:	CCOC(=O)CCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	320.26

## Physical Properties

Property code	Value	Unit	Source
gf	-984.65	kJ/mol	Joback Method
hf	-1326.13	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.972		Crippen Method
mcvol	210.420	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	720.96	K	Joback Method
tc	913.09	K	Joback Method
tf	457.22	K	Joback Method
vc	0.821	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.68	J/mol×K	720.96	Joback Method
cpg	605.42	J/mol×K	752.98	Joback Method
cpg	617.32	J/mol×K	785.00	Joback Method
cpg	628.39	J/mol×K	817.03	Joback Method
cpg	638.64	J/mol×K	849.05	Joback Method
cpg	648.07	J/mol×K	881.07	Joback Method
cpg	656.71	J/mol×K	913.09	Joback Method

# Sources

<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=U381560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381560&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>

# 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>hvp:</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>rlnol:</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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