

# Succinic acid, butyl 4-trifluoromethoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C16H19F3O5/c1-2-3-10-22-14(20)8-9-15(21)23-11-12-4-6-13(7-5-12)24-16(17)
<b>InchiKey:</b>	RZSWCGLWHJDRJK-UHFFFAOYSA-N
<b>Formula:</b>	C16H19F3O5
<b>SMILES:</b>	CCCCOC(=O)CCC(=O)OCc1ccc(OC(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	348.31

## Physical Properties

Property code	Value	Unit	Source
gf	-967.81	kJ/mol	Joback Method
hf	-1367.41	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.752		Crippen Method
mcvol	238.600	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	766.72	K	Joback Method
tc	957.65	K	Joback Method
tf	479.76	K	Joback Method
vc	0.932	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.26	J/mol×K	766.72	Joback Method
cpg	714.75	J/mol×K	798.54	Joback Method
cpg	727.32	J/mol×K	830.36	Joback Method
cpg	738.98	J/mol×K	862.19	Joback Method
cpg	749.75	J/mol×K	894.01	Joback Method
cpg	759.65	J/mol×K	925.83	Joback Method
cpg	768.70	J/mol×K	957.65	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=U381562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381562&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>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>rinp:</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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