

# Succinic acid, heptadecyl 2,3,6-trifluorobenzyl ester

Inchi:	InChI=1S/C28H43F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-34-26(32)19-20-27
InchiKey:	QZLBLBXUCPDFNO-UHFFFAOYSA-N
Formula:	C28H43F3O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]:	500.63

## Physical Properties

Property code	Value	Unit	Source
gf	-783.87	kJ/mol	Joback Method
hf	-1497.06	kJ/mol	Joback Method
hfus	75.96	kJ/mol	Joback Method
hvap	98.04	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.342		Crippen Method
mvol	401.810	ml/mol	McGowan Method
pc	745.29	kPa	Joback Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook
tb	1032.05	K	Joback Method
tc	1281.55	K	Joback Method
tf	615.39	K	Joback Method
vc	1.597	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.07	J/molxK	1032.05	Joback Method
cpg	1406.41	J/molxK	1073.63	Joback Method
cpg	1422.69	J/molxK	1115.22	Joback Method
cpg	1436.97	J/molxK	1156.80	Joback Method
cpg	1449.32	J/molxK	1198.38	Joback Method
cpg	1459.81	J/molxK	1239.97	Joback Method
cpg	1468.51	J/molxK	1281.55	Joback Method

# Sources

<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.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=U381188&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381188&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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