

# Succinic acid, decyl 4-trifluoromethylbenzyl ester

Inchi:	InChI=1S/C22H31F3O4/c1-2-3-4-5-6-7-8-9-16-28-20(26)14-15-21(27)29-17-18-10-12-19
InchiKey:	ABSDHEKPULUSEK-UHFFFAOYSA-N
Formula:	C22H31F3O4
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	416.47

## Physical Properties

Property code	Value	Unit	Source
gf	-812.29	kJ/mol	Joback Method
hf	-1359.03	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	82.07	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.213		Crippen Method
mvol	317.270	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	881.58	K	Joback Method
tc	1080.54	K	Joback Method
tf	525.15	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.44	J/molxK	881.58	Joback Method
cpg	1035.16	J/molxK	914.74	Joback Method
cpg	1049.75	J/molxK	947.90	Joback Method
cpg	1063.24	J/molxK	981.06	Joback Method
cpg	1075.70	J/molxK	1014.22	Joback Method
cpg	1087.16	J/molxK	1047.38	Joback Method
cpg	1097.67	J/molxK	1080.54	Joback Method

# Sources

<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=U382447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382447&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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