

# Succinic acid, 2-fluoro-6-(trifluoromethyl)benzyl undecyl ester

InChI:  
InChIKey:

InChI=1S/C23H32F4O4/c1-2-3-4-5-6-7-8-9-10-16-30-21(28)14-15-22(29)31-17-18-19(23)

QPBSTVSAQUBYRM-UHFFFAOYSA-N

Formula:

C23H32F4O4

SMILES:

CCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]:

448.49

## Physical Properties

Property code	Value	Unit	Source
gf	-1008.31	kJ/mol	Joback Method
hf	-1587.25	kJ/mol	Joback Method
hfus	59.07	kJ/mol	Joback Method
hvap	84.14	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.742		Crippen Method
mvol	333.130	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	908.71	K	Joback Method
tc	1112.56	K	Joback Method
tf	549.53	K	Joback Method
vc	1.325	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.19	J/mol×K	908.71	Joback Method
cpg	1102.05	J/mol×K	942.68	Joback Method
cpg	1116.71	J/mol×K	976.66	Joback Method
cpg	1130.21	J/mol×K	1010.63	Joback Method
cpg	1142.59	J/mol×K	1044.61	Joback Method
cpg	1153.91	J/mol×K	1078.58	Joback Method
cpg	1164.21	J/mol×K	1112.56	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=U381641&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381641&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>h vap:</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>r in pol:</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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