

# 5-Fluoro-2-trifluoromethylbenzoic acid, 2-tridecyl ester

Inchi:	InChI=1S/C21H30F4O2/c1-3-4-5-6-7-8-9-10-11-12-16(2)27-20(26)18-15-17(22)13-14-19
InchiKey:	KKNNCELVWRGWHP-UHFFFAOYSA-N
Formula:	C21H30F4O2
SMILES:	CCCCCCCCCCCC(C)OC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]:	390.46

## Physical Properties

Property code	Value	Unit	Source
gf	-793.67	kJ/mol	Joback Method
hf	-1306.45	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	70.14	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.311		Crippen Method
mcvol	297.510	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	786.22	K	Joback Method
tc	969.32	K	Joback Method
tf	439.83	K	Joback Method
vc	1.183	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.79	J/mol×K	786.22	Joback Method
cpg	933.69	J/mol×K	816.74	Joback Method
cpg	949.60	J/mol×K	847.25	Joback Method
cpg	964.57	J/mol×K	877.77	Joback Method
cpg	978.65	J/mol×K	908.29	Joback Method
cpg	991.86	J/mol×K	938.80	Joback Method
cpg	1004.26	J/mol×K	969.32	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=U338549&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338549&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>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

Latest version available from:

<https://www.cheméo.com/cid/117-857-1/5-Fluoro-2-trifluoromethylbenzoic-acid-2-tridecyl-ester.pdf>

Generated by Cheméo on 2024-05-04 07:24:03.174474634 +0000 UTC m=+17096692.095051949.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.