

# 5-Fluoro-3-trifluoromethylbenzoic acid, tridecyl ester

<b>Inchi:</b>	InChI=1S/C21H30F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-27-20(26)17-14-18(21(23,24)25
<b>InchiKey:</b>	OHIHSNRHBSGROU-UHFFFAOYSA-N
<b>Formula:</b>	C21H30F4O2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1cc(F)cc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	390.46

## Physical Properties

Property code	Value	Unit	Source
gf	-791.23	kJ/mol	Joback Method
hf	-1301.17	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	70.53	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.312		Crippen Method
mcvol	297.510	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	786.66	K	Joback Method
tc	968.61	K	Joback Method
tf	454.83	K	Joback Method
vc	1.188	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.29	J/mol×K	786.66	Joback Method
cpg	933.08	J/mol×K	816.98	Joback Method
cpg	948.90	J/mol×K	847.31	Joback Method
cpg	963.80	J/mol×K	877.63	Joback Method
cpg	977.82	J/mol×K	907.96	Joback Method
cpg	991.00	J/mol×K	938.28	Joback Method
cpg	1003.38	J/mol×K	968.61	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=U338905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338905&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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