

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

<b>Inchi:</b>	InChI=1S/C21H30F4O2/c1-3-5-7-8-9-10-12-17(11-6-4-2)27-20(26)16-13-14-19(22)18(15
<b>InchiKey:</b>	KXNICVDPKRRGJT-UHFFFAOYSA-N
<b>Formula:</b>	C21H30F4O2
<b>SMILES:</b>	CCCCCCCCC(CCCC)OC(=O)c1ccc(F)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	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	2057.00		NIST Webbook
rinpol	2057.00		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>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=U338680&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338680&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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