

# 4-Fluoro-3-trifluoromethylbenzoic acid, undecyl ester

<b>Inchi:</b>	InChI=1S/C19H26F4O2/c1-2-3-4-5-6-7-8-9-10-13-25-18(24)15-11-12-17(20)16(14-15)19
<b>InchiKey:</b>	UMMCIJIARJWEMO-UHFFFAOYSA-N
<b>Formula:</b>	C19H26F4O2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1ccc(F)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	362.40

## Physical Properties

Property code	Value	Unit	Source
gf	-808.07	kJ/mol	Joback Method
hf	-1259.89	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	66.08	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.532		Crippen Method
mcvol	269.330	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	2026.00		NIST Webbook
rinpol	2026.00		NIST Webbook
tb	740.90	K	Joback Method
tc	919.72	K	Joback Method
tf	432.29	K	Joback Method
vc	1.077	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.14	J/mol×K	740.90	Joback Method
cpg	816.18	J/mol×K	770.70	Joback Method
cpg	831.31	J/mol×K	800.51	Joback Method
cpg	845.59	J/mol×K	830.31	Joback Method
cpg	859.04	J/mol×K	860.11	Joback Method
cpg	871.71	J/mol×K	889.92	Joback Method
cpg	883.62	J/mol×K	919.72	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=U338923&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338923&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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