

# 4-Fluoro-2-trifluoromethylbenzoic acid, 5-pentadecyl ester

<b>Inchi:</b>	InChI=1S/C23H34F4O2/c1-3-5-7-8-9-10-11-12-14-19(13-6-4-2)29-22(28)20-16-15-18(24
<b>InchiKey:</b>	OBIGIWNYSJFJF-UHFFFAOYSA-N
<b>Formula:</b>	C23H34F4O2
<b>SMILES:</b>	CCCCCCCCCCC(CCCC)OC(=O)c1ccc(F)cc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	418.51

## Physical Properties

Property code	Value	Unit	Source
gf	-776.83	kJ/mol	Joback Method
hf	-1347.73	kJ/mol	Joback Method
hfus	52.76	kJ/mol	Joback Method
hvap	74.60	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.091		Crippen Method
mcvol	325.690	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpola	2273.00		NIST Webbook
rinpola	2273.00		NIST Webbook
tb	831.98	K	Joback Method
tc	1020.35	K	Joback Method
tf	462.37	K	Joback Method
vc	1.294	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.41	J/molxK	831.98	Joback Method
cpg	1054.07	J/molxK	863.38	Joback Method
cpg	1070.65	J/molxK	894.77	Joback Method
cpg	1086.22	J/molxK	926.17	Joback Method
cpg	1100.83	J/molxK	957.56	Joback Method
cpg	1114.52	J/molxK	988.96	Joback Method
cpg	1127.34	J/molxK	1020.35	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=U338507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338507&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>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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