

# 4-Fluoro-3-trifluoromethylbenzoic acid, 7-tetradecyl ester

<b>Inchi:</b>	InChI=1S/C22H32F4O2/c1-3-5-7-9-11-13-18(12-10-8-6-4-2)28-21(27)17-14-15-20(23)19
<b>InchiKey:</b>	XHYNEMKVKYPFW-UHFFFAOYSA-N
<b>Formula:</b>	C22H32F4O2
<b>SMILES:</b>	CCCCCCCC(CCCCC)OC(=O)c1ccc(F)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	404.48

## Physical Properties

Property code	Value	Unit	Source
gf	-785.25	kJ/mol	Joback Method
hf	-1327.09	kJ/mol	Joback Method
hfus	50.17	kJ/mol	Joback Method
hvap	72.37	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.701		Crippen Method
mvol	311.600	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	809.10	K	Joback Method
tc	994.47	K	Joback Method
tf	451.10	K	Joback Method
vc	1.238	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.20	J/mol×K	809.10	Joback Method
cpg	993.46	J/mol×K	839.99	Joback Method
cpg	1009.71	J/mol×K	870.89	Joback Method
cpg	1024.97	J/mol×K	901.78	Joback Method
cpg	1039.30	J/mol×K	932.68	Joback Method
cpg	1052.75	J/mol×K	963.57	Joback Method
cpg	1065.36	J/mol×K	994.47	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.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>
<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=U338688&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338688&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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