

# 5-Fluoro-2-trifluoromethylbenzoic acid, tetradecyl ester

Inchi:	InChI=1S/C22H32F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-28-21(27)19-17-18(23)14-15
InchiKey:	XXDMTEIXRSJQAU-UHFFFAOYSA-N
Formula:	C22H32F4O2
SMILES:	CCCCCCCCCCCCCOC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]:	404.48

## Physical Properties

Property code	Value	Unit	Source
gf	-782.81	kJ/mol	Joback Method
hf	-1321.81	kJ/mol	Joback Method
hfus	53.69	kJ/mol	Joback Method
hvap	72.76	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.702		Crippen Method
mcvol	311.600	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2307.00		NIST Webbook
rinpol	2307.00		NIST Webbook
tb	809.54	K	Joback Method
tc	994.06	K	Joback Method
tf	466.10	K	Joback Method
vc	1.244	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.71	J/molxK	809.54	Joback Method
cpg	992.89	J/molxK	840.29	Joback Method
cpg	1009.07	J/molxK	871.05	Joback Method
cpg	1024.29	J/molxK	901.80	Joback Method
cpg	1038.60	J/molxK	932.55	Joback Method
cpg	1052.04	J/molxK	963.31	Joback Method
cpg	1064.65	J/molxK	994.06	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=U338750&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338750&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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