

# 2,4,5-Trifluoro-3-methoxybenzoic acid, 4-tetradecyl ester

Inchi:	InChI=1S/C22H33F3O3/c1-4-6-7-8-9-10-11-12-14-16(13-5-2)28-22(26)17-15-18(23)20(2
InchiKey:	OTZSKZIRLCUDAD-UHFFFAOYSA-N
Formula:	C22H33F3O3
SMILES:	CCCCCCCCCCC(CCC)OC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]:	402.49

## Physical Properties

Property code	Value	Unit	Source
gf	-717.54	kJ/mol	Joback Method
hf	-1277.39	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	6.969		Crippen Method
mcvol	315.700	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpola	2409.00		NIST Webbook
rinpola	2409.00		NIST Webbook
tb	845.44	K	Joback Method
tc	1036.30	K	Joback Method
tf	495.36	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.18	J/molxK	845.44	Joback Method
cpg	1015.38	J/molxK	877.25	Joback Method
cpg	1031.47	J/molxK	909.06	Joback Method
cpg	1046.45	J/molxK	940.87	Joback Method
cpg	1060.34	J/molxK	972.68	Joback Method
cpg	1073.15	J/molxK	1004.49	Joback Method
cpg	1084.91	J/molxK	1036.30	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=U338463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338463&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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