

# 3-Chloro2-fluorobenzoic acid, 6-tetradecyl ester

Inchi:	InChI=1S/C21H32ClFO2/c1-3-5-7-8-9-11-14-17(13-10-6-4-2)25-21(24)18-15-12-16-19(2)
InchiKey:	GELZNXXPISJJKK-UHFFFAOYSA-N
Formula:	C21H32ClFO2
SMILES:	CCCCCCCC(CCCCC)OC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]:	370.93

## Physical Properties

Property code	Value	Unit	Source
gf	-224.01	kJ/mol	Joback Method
hf	-725.11	kJ/mol	Joback Method
hfus	49.95	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.335		Crippen Method
mvol	304.440	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	829.07	K	Joback Method
tc	1024.31	K	Joback Method
tf	465.56	K	Joback Method
vc	1.188	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.79	J/molxK	829.07	Joback Method
cpg	940.76	J/molxK	861.61	Joback Method
cpg	956.68	J/molxK	894.15	Joback Method
cpg	971.57	J/molxK	926.69	Joback Method
cpg	985.47	J/molxK	959.23	Joback Method
cpg	998.41	J/molxK	991.77	Joback Method
cpg	1010.42	J/molxK	1024.31	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=U338649&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338649&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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