

# 3-Chloro2-fluorobenzoic acid, 2-tridecyl ester

<b>Inchi:</b>	InChI=1S/C20H30ClFO2/c1-3-4-5-6-7-8-9-10-11-13-16(2)24-20(23)17-14-12-15-18(21)1
<b>InchiKey:</b>	RBZBUXZBUMBEBEW-UHFFFAOYSA-N
<b>Formula:</b>	C20H30ClFO2
<b>SMILES:</b>	CCCCCCCCCCCC(C)OC(=O)c1cccc(Cl)c1F
<b>Mol. weight [g/mol]:</b>	356.90

## Physical Properties

Property code	Value	Unit	Source
gf	-232.43	kJ/mol	Joback Method
hf	-704.47	kJ/mol	Joback Method
hfus	47.36	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.945		Crippen Method
mvol	290.350	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	806.19	K	Joback Method
tc	1000.51	K	Joback Method
tf	454.29	K	Joback Method
vc	1.133	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.64	J/mol×K	806.19	Joback Method
cpg	881.34	J/mol×K	838.58	Joback Method
cpg	897.01	J/mol×K	870.96	Joback Method
cpg	911.70	J/mol×K	903.35	Joback Method
cpg	925.42	J/mol×K	935.73	Joback Method
cpg	938.22	J/mol×K	968.12	Joback Method
cpg	950.12	J/mol×K	1000.51	Joback Method

# Sources

<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=U338642&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338642&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvpap:</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>rinppl:</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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