

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

Inchi:	InChI=1S/C22H34ClFO2/c1-3-5-7-8-9-10-12-15-18(14-11-6-4-2)26-22(25)19-16-13-17-20
InchiKey:	XRFKUCZZWKPQTF-UHFFFAOYSA-N
Formula:	C22H34ClFO2
SMILES:	CCCCCCCCC(CCCCC)OC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]:	384.96

## Physical Properties

Property code	Value	Unit	Source
gf	-215.59	kJ/mol	Joback Method
hf	-745.75	kJ/mol	Joback Method
hfus	52.54	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.726		Crippen Method
mvol	318.530	ml/mol	McGowan Method
pc	1070.06	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	851.95	K	Joback Method
tc	1048.82	K	Joback Method
tf	476.83	K	Joback Method
vc	1.244	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.73	J/mol×K	851.95	Joback Method
cpg	1000.99	J/mol×K	884.76	Joback Method
cpg	1017.15	J/mol×K	917.57	Joback Method
cpg	1032.24	J/mol×K	950.39	Joback Method
cpg	1046.31	J/mol×K	983.20	Joback Method
cpg	1059.38	J/mol×K	1016.01	Joback Method
cpg	1071.50	J/mol×K	1048.82	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=U338653&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338653&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>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>rlnol:</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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