

# 3-Fluorobenzoic acid, 8-chlorooctyl ester

**Inchi:** InChI=1S/C15H20ClFO2/c16-10-5-3-1-2-4-6-11-19-15(18)13-8-7-9-14(17)12-13/h7-9,12H  
**InchiKey:** YZSYZDFQZYCLBT-UHFFFAOYSA-N  
**Formula:** C15H20ClFO2  
**SMILES:** O=C(OCCCCCCCCCl)c1cccc(F)c1  
**Mol. weight [g/mol]:** 286.77

## Physical Properties

Property code	Value	Unit	Source
gf	-262.46	kJ/mol	Joback Method
hf	-584.52	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.562		Crippen Method
mvol	219.900	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	687.25	K	Joback Method
tc	881.81	K	Joback Method
tf	400.42	K	Joback Method
vc	0.859	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.58	J/mol×K	687.25	Joback Method
cpg	598.51	J/mol×K	719.68	Joback Method
cpg	612.59	J/mol×K	752.10	Joback Method
cpg	625.83	J/mol×K	784.53	Joback Method
cpg	638.27	J/mol×K	816.96	Joback Method
cpg	649.93	J/mol×K	849.38	Joback Method
cpg	660.82	J/mol×K	881.81	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=U355666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355666&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>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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