

# 3-Chlorobenzoic acid, pentafluorobenzyl ester

**Inchi:** InChI=1S/C14H6ClF5O2/c15-7-3-1-2-6(4-7)14(21)22-5-8-9(16)11(18)13(20)12(19)10(8)1  
**InchiKey:** OAAVKYAFTYDFGI-UHFFFAOYSA-N  
**Formula:** C14H6ClF5O2  
**SMILES:** O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1cccc(Cl)c1  
**Mol. weight [g/mol]:** 336.64

## Physical Properties

Property code	Value	Unit	Source
gf	-985.86	kJ/mol	Joback Method
hf	-1169.14	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.393		Crippen Method
mcvol	189.130	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpola	1850.00		NIST Webbook
tb	713.03	K	Joback Method
tc	915.85	K	Joback Method
tf	480.53	K	Joback Method
vc	0.766	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.70	J/mol×K	713.03	Joback Method
cpg	482.86	J/mol×K	746.83	Joback Method
cpg	492.33	J/mol×K	780.64	Joback Method
cpg	501.12	J/mol×K	814.44	Joback Method
cpg	509.23	J/mol×K	848.24	Joback Method
cpg	516.66	J/mol×K	882.04	Joback Method
cpg	523.44	J/mol×K	915.85	Joback Method

# Sources

<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=U357396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357396&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>
<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>

# 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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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