

# 2,3,4-Trifluorobenzoic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C13H6ClF3O2/c14-7-1-3-8(4-2-7)19-13(18)9-5-6-10(15)12(17)11(9)16/h1-6H
InchiKey:	GPXLYOWAAILFAD-UHFFFAOYSA-N
Formula:	C13H6ClF3O2
SMILES:	O=C(Oc1ccc(Cl)cc1)c1ccc(F)c(F)c1F
Mol. weight [g/mol]:	286.63

## Physical Properties

Property code	Value	Unit	Source
gf	-585.40	kJ/mol	Joback Method
hf	-733.34	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.976		Crippen Method
mcvol	171.500	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	681.65	K	Joback Method
tc	903.02	K	Joback Method
tf	443.04	K	Joback Method
vc	0.674	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.71	J/mol×K	681.65	Joback Method
cpg	420.52	J/mol×K	718.55	Joback Method
cpg	430.53	J/mol×K	755.44	Joback Method
cpg	439.75	J/mol×K	792.34	Joback Method
cpg	448.20	J/mol×K	829.23	Joback Method
cpg	455.90	J/mol×K	866.13	Joback Method
cpg	462.87	J/mol×K	903.02	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=U308031&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308031&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>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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