

# 2-Trifluoromethylbenzoic acid, 4-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C14H8ClF3O2/c15-9-5-7-10(8-6-9)20-13(19)11-3-1-2-4-12(11)14(16,17)18/h1-
<b>InchiKey:</b>	JKWUCDALVOYHGH-UHFFFAOYSA-N
<b>Formula:</b>	C14H8ClF3O2
<b>SMILES:</b>	O=C(Oc1ccc(Cl)cc1)c1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	300.66

## Physical Properties

Property code	Value	Unit	Source
gf	-554.88	kJ/mol	Joback Method
hf	-739.79	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.578		Crippen Method
mvol	185.590	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	691.34	K	Joback Method
tc	919.23	K	Joback Method
tf	431.69	K	Joback Method
vc	0.720	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.51	J/mol×K	691.34	Joback Method
cpg	477.56	J/mol×K	729.32	Joback Method
cpg	488.56	J/mol×K	767.30	Joback Method
cpg	498.59	J/mol×K	805.28	Joback Method
cpg	507.70	J/mol×K	843.27	Joback Method
cpg	515.95	J/mol×K	881.25	Joback Method
cpg	523.41	J/mol×K	919.23	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307669&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307669&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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