

# 2-Fluoro-6-trifluoromethylbenzoic acid, 3,4-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C14H6Cl2F4O2/c15-9-5-4-7(6-10(9)16)22-13(21)12-8(14(18,19)20)2-1-3-11(12)
<b>InchiKey:</b>	RVNSBKSHHZXGMD-UHFFFAOYSA-N
<b>Formula:</b>	C14H6Cl2F4O2
<b>SMILES:</b>	O=C(Oc1ccc(Cl)c(Cl)c1)c1c(F)cccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	353.10

## Physical Properties

Property code	Value	Unit	Source
gf	-780.88	kJ/mol	Joback Method
hf	-974.58	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.370		Crippen Method
mcvol	199.600	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinqol	1974.00		NIST Webbook
tb	738.00	K	Joback Method
tc	960.76	K	Joback Method
tf	487.24	K	Joback Method
vc	0.786	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.48	J/mol×K	738.00	Joback Method
cpg	502.52	J/mol×K	775.13	Joback Method
cpg	511.67	J/mol×K	812.25	Joback Method
cpg	520.00	J/mol×K	849.38	Joback Method
cpg	527.53	J/mol×K	886.51	Joback Method
cpg	534.33	J/mol×K	923.63	Joback Method
cpg	540.44	J/mol×K	960.76	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357700&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357700&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>hvap:</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>rinpola:</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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