

# 2,5-Di(trifluoromethyl)benzoic acid, 3,4-dichlorophenyl ester

**Inchi:** InChI=1S/C15H6Cl2F6O2/c16-11-4-2-8(6-12(11)17)25-13(24)9-5-7(14(18,19)20)1-3-10(S)  
**InchiKey:** GFJRUSPBZSANSO-UHFFFAOYSA-N  
**Formula:** C15H6Cl2F6O2  
**SMILES:** O=C(Oc1ccc(Cl)c(Cl)c1)c1cc(C(F)(F)F)ccc1C(F)(F)F  
**Mol. weight [g/mol]:** 403.10

## Physical Properties

Property code	Value	Unit	Source
gf	-1159.24	kJ/mol	Joback Method
hf	-1396.19	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	66.62	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.250		Crippen Method
mvol	217.230	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook
tb	756.19	K	Joback Method
tc	969.40	K	Joback Method
tf	502.11	K	Joback Method
vc	0.868	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.10	J/molxK	756.19	Joback Method
cpg	571.81	J/molxK	791.73	Joback Method
cpg	580.65	J/molxK	827.26	Joback Method
cpg	588.69	J/molxK	862.80	Joback Method
cpg	595.99	J/molxK	898.33	Joback Method
cpg	602.62	J/molxK	933.87	Joback Method
cpg	608.64	J/molxK	969.40	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357748&amp;Units=SI</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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