

# 2,5-Di(trifluoromethyl)benzoic acid, phenyl ester

Inchi:	InChI=1S/C15H8F6O2/c16-14(17,18)9-6-7-12(15(19,20)21)11(8-9)13(22)23-10-4-2-1-3-5
InchiKey:	LGJLJNQWHFIDAU-UHFFFAOYSA-N
Formula:	C15H8F6O2
SMILES:	O=C(Oc1ccccc1)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	334.21

## Physical Properties

Property code	Value	Unit	Source
gf	-1116.12	kJ/mol	Joback Method
hf	-1341.77	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.943		Crippen Method
mcvol	192.750	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinsol	1543.00		NIST Webbook
tb	671.37	K	Joback Method
tc	876.20	K	Joback Method
tf	417.23	K	Joback Method
vc	0.769	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.96	J/molxK	671.37	Joback Method
cpg	531.33	J/molxK	705.51	Joback Method
cpg	542.68	J/molxK	739.65	Joback Method
cpg	553.08	J/molxK	773.79	Joback Method
cpg	562.61	J/molxK	807.93	Joback Method
cpg	571.31	J/molxK	842.06	Joback Method
cpg	579.27	J/molxK	876.20	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=U357741&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357741&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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