

# 2-Trifluoromethylbenzoic acid, phenyl ester

<b>Inchi:</b>	InChI=1S/C14H9F3O2/c15-14(16,17)12-9-5-4-8-11(12)13(18)19-10-6-2-1-3-7-10/h1-9H
<b>InchiKey:</b>	ZHFBGJIMMTZRIC-UHFFFAOYSA-N
<b>Formula:</b>	C14H9F3O2
<b>SMILES:</b>	O=C(Oc1ccccc1)c1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	266.22

## Physical Properties

Property code	Value	Unit	Source
gf	-533.32	kJ/mol	Joback Method
hf	-712.58	kJ/mol	Joback Method
hfus	24.32	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.925		Crippen Method
mvol	173.350	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	648.93	K	Joback Method
tc	872.96	K	Joback Method
tf	389.25	K	Joback Method
vc	0.670	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.47	J/mol×K	648.93	Joback Method
cpg	455.97	J/mol×K	686.27	Joback Method
cpg	468.36	J/mol×K	723.61	Joback Method
cpg	479.70	J/mol×K	760.95	Joback Method
cpg	490.06	J/mol×K	798.29	Joback Method
cpg	499.49	J/mol×K	835.62	Joback Method
cpg	508.07	J/mol×K	872.96	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U299009&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299009&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>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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