

# 3-Trifluoromethylbenzoic acid, 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C15H11F3O2/c1-10-4-2-7-13(8-10)20-14(19)11-5-3-6-12(9-11)15(16,17)18/h2
<b>InchiKey:</b>	RLXDEQCMJWEQDP-UHFFFAOYSA-N
<b>Formula:</b>	C15H11F3O2
<b>SMILES:</b>	Cc1cccc(OC(=O)c2cccc(C(F)(F)F)c2)c1
<b>Mol. weight [g/mol]:</b>	280.24

## Physical Properties

Property code	Value	Unit	Source
gf	-534.53	kJ/mol	Joback Method
hf	-744.69	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.233		Crippen Method
mvol	187.440	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	676.79	K	Joback Method
tc	897.71	K	Joback Method
tf	413.04	K	Joback Method
vc	0.727	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.84	J/molxK	676.79	Joback Method
cpg	505.60	J/molxK	713.61	Joback Method
cpg	518.28	J/molxK	750.43	Joback Method
cpg	529.94	J/molxK	787.25	Joback Method
cpg	540.64	J/molxK	824.07	Joback Method
cpg	550.43	J/molxK	860.89	Joback Method
cpg	559.37	J/molxK	897.71	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=U307676&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307676&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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