

# 2,3,4-Trifluorobenzoic acid, tridec-2-ynyl ester

<b>Inchi:</b>	InChI=1S/C20H25F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-25-20(24)16-13-14-17(21)19(23)
<b>InchiKey:</b>	NJALBNFKWCOINX-UHFFFAOYSA-N
<b>Formula:</b>	C20H25F3O2
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)c1ccc(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	354.41

## Physical Properties

Property code	Value	Unit	Source
gf	-414.51	kJ/mol	Joback Method
hf	-814.84	kJ/mol	Joback Method
hfus	55.58	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.795		Crippen Method
mcvol	273.050	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinsol	2265.40		NIST Webbook
tb	781.72	K	Joback Method
tc	972.44	K	Joback Method
tf	559.17	K	Joback Method
vc	1.087	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.05	J/mol×K	781.72	Joback Method
cpg	815.90	J/mol×K	813.51	Joback Method
cpg	830.84	J/mol×K	845.29	Joback Method
cpg	844.88	J/mol×K	877.08	Joback Method
cpg	858.04	J/mol×K	908.86	Joback Method
cpg	870.34	J/mol×K	940.65	Joback Method
cpg	881.82	J/mol×K	972.44	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=U292560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292560&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>

# 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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