

# 4-(Trifluoromethyl)benzoic acid, pent-2-en-4-ynyl ester

<b>Inchi:</b>	InChI=1S/C13H9F3O2/c1-2-3-4-9-18-12(17)10-5-7-11(8-6-10)13(14,15)16/h1,3-8H,9H2
<b>InchiKey:</b>	UJVYDZIZKFKVHB-UHFFFAOYSA-N
<b>Formula:</b>	C13H9F3O2
<b>SMILES:</b>	C#CC=CCOC(=O)c1ccc(C(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	254.20

## Physical Properties

Property code	Value	Unit	Source
gf	-350.86	kJ/mol	Joback Method
hf	-519.35	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.052		Crippen Method
mcvol	170.120	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinsol	1454.00		NIST Webbook
tb	593.65	K	Joback Method
tc	802.09	K	Joback Method
tf	393.45	K	Joback Method
vc	0.664	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.28	J/mol×K	593.65	Joback Method
cpg	421.76	J/mol×K	628.39	Joback Method
cpg	433.33	J/mol×K	663.13	Joback Method
cpg	444.05	J/mol×K	697.87	Joback Method
cpg	453.98	J/mol×K	732.61	Joback Method
cpg	463.18	J/mol×K	767.35	Joback Method
cpg	471.71	J/mol×K	802.09	Joback Method

# Sources

<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=U299440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299440&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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