

# 3-(Trifluoromethoxy)cinnamic acid

<b>Inchi:</b>	InChI=1S/C10H7F3O3/c11-10(12,13)16-8-3-1-2-7(6-8)4-5-9(14)15/h1-6H,(H,14,15)/b5-4
<b>InchiKey:</b>	CLKZZEYGXRWYNI-SNAWJCMRSA-N
<b>Formula:</b>	C10H7F3O3
<b>SMILES:</b>	O=C(O)C=Cc1cccc(OC(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	232.16
<b>CAS:</b>	168833-80-5

## Physical Properties

Property code	Value	Unit	Source
gf	-736.01	kJ/mol	Joback Method
hf	-901.56	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.683		Crippen Method
mcvol	142.320	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	627.07	K	Joback Method
tc	819.11	K	Joback Method
tf	373.49	K	Joback Method
vc	0.553	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.73	J/molxK	627.07	Joback Method
cpg	365.96	J/molxK	659.08	Joback Method
cpg	374.55	J/molxK	691.08	Joback Method
cpg	382.54	J/molxK	723.09	Joback Method
cpg	389.96	J/molxK	755.10	Joback Method
cpg	396.85	J/molxK	787.10	Joback Method
cpg	403.25	J/molxK	819.11	Joback Method

# Sources

<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>
<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=C168833805&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C168833805&amp;Units=SI</a>
<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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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