

# Homovanillic acid, TFA-ME

<b>Inchi:</b>	InChI=1S/C12H11F3O5/c1-18-9-5-7(6-10(16)19-2)3-4-8(9)20-11(17)12(13,14)15/h3-5H,6
<b>InchiKey:</b>	VBXONNMYYFIPNO-UHFFFAOYSA-N
<b>Formula:</b>	C12H11F3O5
<b>SMILES:</b>	<chem>COC(=O)Cc1ccc(OC(=O)C(F)(F)F)c(OC)c1</chem>
<b>Mol. weight [g/mol]:</b>	292.21

## Physical Properties

Property code	Value	Unit	Source
gf	-1011.12	kJ/mol	Joback Method
hf	-1296.32	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	62.88	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.878		Crippen Method
mcvol	182.240	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
tb	680.18	K	Joback Method
tc	876.29	K	Joback Method
tf	447.20	K	Joback Method
vc	0.709	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.66	J/molxK	680.18	Joback Method
cpg	499.31	J/molxK	712.87	Joback Method
cpg	510.22	J/molxK	745.55	Joback Method
cpg	520.38	J/molxK	778.24	Joback Method
cpg	529.81	J/molxK	810.92	Joback Method
cpg	538.51	J/molxK	843.61	Joback Method
cpg	546.47	J/molxK	876.29	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R387185&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R387185&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>
<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>

# 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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