

# Homovanillic acid, acetyl, DTFMBz

**Inchi:** InChI=1S/C20H16F6O5/c1-11(27)31-16-4-3-12(7-17(16)29-2)8-18(28)30-10-13-5-14(19)  
**InchiKey:** RGRLBRRFRWDYKA-UHFFFAOYSA-N  
**Formula:** C20H16F6O5  
**SMILES:** COc1cc(CC(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)ccc1OC(C)=O  
**Mol. weight [g/mol]:** 450.33

## Physical Properties

Property code	Value	Unit	Source
gf	-1432.20	kJ/mol	Joback Method
hf	-1844.93	kJ/mol	Joback Method
hfus	44.50	kJ/mol	Joback Method
hvap	80.54	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.944		Crippen Method
mvol	276.510	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	894.44	K	Joback Method
tc	1102.66	K	Joback Method
tf	593.01	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.28	J/mol×K	894.44	Joback Method
cpg	861.41	J/mol×K	929.14	Joback Method
cpg	871.46	J/mol×K	963.85	Joback Method
cpg	880.48	J/mol×K	998.55	Joback Method
cpg	888.50	J/mol×K	1033.25	Joback Method
cpg	895.58	J/mol×K	1067.96	Joback Method
cpg	901.75	J/mol×K	1102.66	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=R538982&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R538982&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>
<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>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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