

# Hydroquinone, TFA-HFB

<b>Inchi:</b>	InChI=1S/C12H4F10O4/c13-9(14,11(18,19)12(20,21)22)7(23)25-5-1-3-6(4-2-5)26-8(24)1
<b>InchiKey:</b>	RKZQEXQZJYVYMO-UHFFFAOYSA-N
<b>Formula:</b>	C12H4F10O4
<b>SMILES:</b>	O=C(Oc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	402.14

## Physical Properties

Property code	Value	Unit	Source
gf	-2251.64	kJ/mol	Joback Method
hf	-2551.65	kJ/mol	Joback Method
hfus	27.21	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.893		Crippen Method
mcvol	188.760	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinsol	1101.00		NIST Webbook
tb	637.98	K	Joback Method
tc	811.02	K	Joback Method
tf	423.84	K	Joback Method
vc	0.783	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.58	J/mol×K	637.98	Joback Method
cpg	540.46	J/mol×K	666.82	Joback Method
cpg	549.53	J/mol×K	695.66	Joback Method
cpg	557.83	J/mol×K	724.50	Joback Method
cpg	565.43	J/mol×K	753.34	Joback Method
cpg	572.36	J/mol×K	782.18	Joback Method
cpg	578.68	J/mol×K	811.02	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R335401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R335401&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>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>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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