

# (6S,9R)-Vomifolyl 9-O-«beta»-D-glucopyranoside, TFA

<b>Inchi:</b>	InChI=1S/C29H25F15O13/c1-10-7-12(45)8-23(3,4)24(10,57-22(50)29(42,43)44)6-5-11(2
<b>InchiKey:</b>	MIHGVEFQWWLBUMI-HNVNEJNSSA-N
<b>Formula:</b>	C29H25F15O13
<b>SMILES:</b>	CC1=CC(=O)CC(C)(C)C1(C=CC(C)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC
<b>Mol. weight [g/mol]:</b>	866.48

## Physical Properties

Property code	Value	Unit	Source
gf	-4100.48	kJ/mol	Joback Method
hf	-5057.54	kJ/mol	Joback Method
hfus	76.55	kJ/mol	Joback Method
hvap	115.89	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	4.990		Crippen Method
mvol	466.210	ml/mol	McGowan Method
pc	648.45	kPa	Joback Method
rinpol	2317.00		NIST Webbook
tb	1358.55	K	Joback Method
tc	1820.86	K	Joback Method
tf	949.92	K	Joback Method
vc	1.857	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1886.41	J/molxK	1358.55	Joback Method
cpg	1948.01	J/molxK	1435.60	Joback Method
cpg	2018.74	J/molxK	1512.65	Joback Method
cpg	2100.76	J/molxK	1589.71	Joback Method
cpg	2196.21	J/molxK	1666.76	Joback Method
cpg	2307.24	J/molxK	1743.81	Joback Method
cpg	2435.99	J/molxK	1820.86	Joback Method

# Sources

<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>
<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=R330411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R330411&amp;Units=SI</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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