

# «alpha»-Hydroxycerotic acid, HFB-Me

<b>Inchi:</b>	InChI=1S/C31H53F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-2
<b>InchiKey:</b>	FBBMARXQNWWHNY-UHFFFAOYSA-N
<b>Formula:</b>	C31H53F7O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)OC
<b>Mol. weight [g/mol]:</b>	622.74

## Physical Properties

Property code	Value	Unit	Source
gf	-1615.29	kJ/mol	Joback Method
hf	-2577.07	kJ/mol	Joback Method
hfus	77.41	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-11.93		Crippen Method
logp	10.896		Crippen Method
mcvol	474.920	ml/mol	McGowan Method
pc	527.99	kPa	Joback Method
rinpol	2946.00		NIST Webbook
rinpol	2946.00		NIST Webbook
tb	1046.02	K	Joback Method
tc	1349.51	K	Joback Method
tf	579.84	K	Joback Method
vc	1.907	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1715.12	J/mol×K	1046.02	Joback Method
cpg	1742.28	J/mol×K	1096.60	Joback Method
cpg	1767.17	J/mol×K	1147.18	Joback Method
cpg	1790.17	J/mol×K	1197.77	Joback Method
cpg	1811.65	J/mol×K	1248.35	Joback Method
cpg	1832.00	J/mol×K	1298.93	Joback Method
cpg	1851.59	J/mol×K	1349.51	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=R134248&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R134248&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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