

# «beta»-Betulinal

<b>Inchi:</b>	InChI=1S/C28H44O2/c1-18(2)21-10-13-28(17-29)15-14-26(4)22(24(21)28)6-7-23-25(3)1
<b>InchiKey:</b>	HMSBMCRNPXWBSB-WKRZZJMVSA-N
<b>Formula:</b>	C28H44O2
<b>SMILES:</b>	<chem>C=C(C)C1CCC2(C=O)CCC3(C)C(CCC4C5(C)CCC(O)CC5CCC43C)C12</chem>
<b>Mol. weight [g/mol]:</b>	412.65

## Physical Properties

Property code	Value	Unit	Source
gf	198.47	kJ/mol	Joback Method
hf	-457.12	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	95.18	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.568		Crippen Method
mvol	354.220	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
ripol	2193.00		NIST Webbook
tb	1014.37	K	Joback Method
tc	1254.62	K	Joback Method
tf	635.40	K	Joback Method
vc	1.345	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.34	J/mol×K	1014.37	Joback Method
cpg	1478.70	J/mol×K	1054.41	Joback Method
cpg	1528.93	J/mol×K	1094.45	Joback Method
cpg	1583.70	J/mol×K	1134.50	Joback Method
cpg	1643.66	J/mol×K	1174.54	Joback Method
cpg	1709.47	J/mol×K	1214.58	Joback Method
cpg	1781.81	J/mol×K	1254.62	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=R560875&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R560875&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>ripol:</b>	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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