Betulin

Other names:	3aH-Cyclopenta[a]chrysene, lup-20(29)-ene-3,28-diol deriv.
	Betulenol
	Betuline
	Betulinol
	Betulol
	Lup-20(29)-ene-3,28-diol, (3«beta»)-
	Lup-20(29)-ene-3,28-diol, (3Â«betaÂ»)-
	Lup-20(29)-ene-3«beta»,28-diol
	Lup-20(29)-ene-3Â«betaÂ»,28-diol
	Lup-20(30)-ene-3«beta»,28-diol
	Lup-20(30)-ene-3Â«betaÂ»,28-diol
	NSC 4644
	Trochol
Inchi:	InChI=1S/C30H50O2/c1-19(2)20-10-15-30(18-31)17-16-28(6)21(25(20)30)8-9-23-27(5)1
InchiKey:	FVWJYYTZTCVBKE-RJBYIQQZSA-N
Formula:	C30H50O2
SMILES:	C=C(C)C1CCC2(CO)CCC3(C)C(CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]:	442.72
CAS:	473-98-3

Physical Properties

Property code	Value	Unit	Source
gf	164.81	kJ/mol	Joback Method
hf	-570.15	kJ/mol	Joback Method
hfus	52.06	kJ/mol	Solubilities of betulin in chloroform + methanol mixed solvents at T = (278.2, 288.2, 293.2, 298.2, 308.2 and 313.2) K
hfus	55.17	kJ/mol	Experimental solubility for betulin and estrone in various solvents within the temperature range T = (293.2 to 328.2) K
hvap	108.13	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.997		Crippen Method
mcvol	386.700	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method

rinpol	3760.50		NIST Webbook
rinpol	3760.50		NIST Webbook
tb	1099.22	K	Joback Method
tc	1346.06	K	Joback Method
tf	696.42	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1701.77	J/mol×K	1099.22	Joback Method
cpg	1769.74	J/mol×K	1140.36	Joback Method
cpg	1844.72	J/mol×K	1181.50	Joback Method
cpg	1927.56	J/mol×K	1222.64	Joback Method
cpg	2019.10	J/mol×K	1263.78	Joback Method
cpg	2120.19	J/mol×K	1304.92	Joback Method
cpg	2231.67	J/mol×K	1346.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473983&Units=SI
Experimental solubility for betulin and estrone in various solvents within the temperature range T = (293.2 to 328.2) K:	https://www.doi.org/10.1016/j.jct.2016.02.006
Solubilities of Betulin in Pyruvic Acid + Water and Ethanol + Water Mixed Organic Solvents at Different Temperatures:	https://www.doi.org/10.1021/je700069g
Experimental Determination of Solubilities of Betulin in Acetone + Water and Ethanol + Water Mixed Solvents at T = (278.2, 288.2, 293.2, 298.2, 303.2, and 313.2) K:	https://www.doi.org/10.1021/je7004177
Solubilities of betulin and betulinic acid in sodium hydroxide aqueous solutions at T = (278.2, 288.2, 293.2, 298.2, 303.2, and 313.2) K:	https://www.doi.org/10.1016/j.jct.2013.07.014
Solubilities of betulin in chloroform + methanol mixed solvents at T = (278.2, 288.2, 293.2, 298.2, 308.2, and 318.2) K:	https://www.doi.org/10.1016/j.fluid.2008.02.013
Solubility of betulin at temperatures from 288.2 K to 323.2 K:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume