Lupeol

Other names:	Lup-20(29)-en-3-ol, (3«beta»)-
	Lup-20(29)-en-3«beta»-ol
	«beta»-Viscol
	Clerodol
	Fagarasterol
	Fagarsterol
	Lupenol
	Monogynol B
	Triterpene lupeol
	1H-Cyclopenta[a]chrysene, lup-20(29)-en-3-ol deriv.
	3«beta»-Lup-20(29)-en-3-ol
	NSC 90487
	«beta»-Lupeol
Inchi:	InChI=1S/C30H50O/c1-19(2)20-11-14-27(5)17-18-29(7)21(25(20)27)9-10-23-28(6)15-13
InchiKey:	MQYXUWHLBZFQQO-RJBYIQQZSA-N
Formula:	C30H50O
SMILES:	C=C(C)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]:	426.72
CAS:	545-47-1

Physical Properties

Property code	Value	Unit	Source
gf	301.63	kJ/mol	Joback Method
hf	-417.92	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	91.45	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.025		Crippen Method
mcvol	380.830	ml/mol	McGowan Method
pc	1019.43	kPa	Joback Method
rinpol	3270.00		NIST Webbook
rinpol	3270.00		NIST Webbook
tb	1007.04	K	Joback Method
tc	1245.95	K	Joback Method
tf	635.60	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1551.91	J/mol×K	1007.04	Joback Method
cpg	1605.28	J/mol×K	1046.86	Joback Method
cpg	1663.42	J/mol×K	1086.68	Joback Method
cpg	1727.09	J/mol×K	1126.50	Joback Method
cpg	1797.05	J/mol×K	1166.31	Joback Method
cpg	1874.08	J/mol×K	1206.13	Joback Method
cpg	1958.92	J/mol×K	1245.95	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C545471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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