3«beta»-Acetoxy-30-norlupan-20-one

Inchi: InChI=1S/C31H50O3/c1-19(32)21-11-14-28(5)17-18-30(7)22(26(21)28)9-10-24-29(6)15-
InchiKey: CACUJZIALZRTTC-LEAOFOMISA-N
Formula: C31H50O3
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CCC2C4C(C(C)=O)CCC4(C)CCC23C)C1(C)C
Mol. weight [g/mol]: 470.73

Physical Properties

Property code	Value	Unit	Source
gf	4.74	kJ/mol	Joback Method
hf	-759.35	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.609		Crippen Method
mcvol	402.360	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	3550.00		NIST Webbook
tb	1071.34	K	Joback Method
tc	1322.70	K	Joback Method
tf	723.86	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1697.38	J/mol×K	1071.34	Joback Method
cpg	1760.79	J/mol×K	1113.23	Joback Method
cpg	1830.35	J/mol×K	1155.13	Joback Method
cpg	1906.93	J/mol×K	1197.02	Joback Method
cpg	1991.35	J/mol×K	1238.91	Joback Method
cpg	2084.48	J/mol×K	1280.80	Joback Method
cpg	2187.15	J/mol×K	1322.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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