(20RS)-3«beta»-Acetoxylupan-29-al

Inchi: InChI=1S/C32H52O3/c1-20(19-33)22-11-14-29(5)17-18-31(7)23(27(22)29)9-10-25-30(6)
InchiKey: UBKAWVIUQSENAF-PTSIISETSA-N
Formula: C32H52O3
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CCC2C4C(C(C)C=O)CCC4(C)CCC23C)C1(C)C
Mol. weight [g/mol]: 484.75

Physical Properties

Property code	Value	Unit	Source
gf	40.12	kJ/mol	Joback Method
hf	-758.27	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	95.30	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	7.854		Crippen Method
mcvol	416.450	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	3660.00		NIST Webbook
rinpol	3660.00		NIST Webbook
tb	1088.57	K	Joback Method
tc	1339.95	K	Joback Method
tf	712.20	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1778.31	J/mol×K	1088.57	Joback Method
cpg	1844.89	J/mol×K	1130.47	Joback Method
cpg	1917.94	J/mol×K	1172.36	Joback Method
cpg	1998.33	J/mol×K	1214.26	Joback Method
cpg	2086.92	J/mol×K	1256.16	Joback Method
cpg	2184.56	J/mol×K	1298.05	Joback Method
cpg	2292.10	J/mol×K	1339.95	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583318&Units=SI

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