Acetyl betulinaldehyde

Inchi: InChI=1S/C32H50O3/c1-20(2)22-11-16-32(19-33)18-17-30(7)23(27(22)32)9-10-25-29(6)
InchiKey: VATQYYFSJMNJAL-UHFFFAOYSA-N
Formula: C32H50O3
SMILES: C=C(C)C1CCC2(C=O)CCC3(C)C(CCC4C5(C)CCC(OC(C)=O)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]: 482.74
CAS: 27570-21-4

Physical Properties

Property code	Value	Unit	Source
gf	121.85	kJ/mol	Joback Method
hf	-637.35	kJ/mol	Joback Method
hfus	34.13	kJ/mol	Joback Method
hvap	95.10	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.775		Crippen Method
mcvol	412.150	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	3744.10		NIST Webbook
rinpol	3744.10		NIST Webbook
tb	1085.57	K	Joback Method
tc	1337.99	K	Joback Method
tf	711.48	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1743.80	J/mol×K	1085.57	Joback Method
cpg	1810.13	J/mol×K	1127.64	Joback Method
cpg	1883.10	J/mol×K	1169.71	Joback Method
cpg	1963.57	J/mol×K	1211.78	Joback Method
cpg	2052.44	J/mol×K	1253.85	Joback Method
cpg	2150.56	J/mol×K	1295.92	Joback Method
cpg	2258.83	J/mol×K	1337.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27570214&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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