10A-5,24-Cucurbitadienol acetate

Inchi: InChI=1S/C32H52O2/c1-21(2)11-10-12-22(3)24-17-18-32(9)27-15-13-25-26(30(27,7)19-
InchiKey: WIQKDJRPJQQUQD-DUJBNXGOSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2C(=CCC3C2(C)CCC2(C)C(C(C)CCC=C(C)C)CCC32C)C1(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	203.90	kJ/mol	Joback Method
hf	-560.15	kJ/mol	Joback Method
hfus	38.76	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.906		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	832.90	kPa	Joback Method
rinpol	3286.00		NIST Webbook
tb	1046.18	K	Joback Method
tc	1287.25	K	Joback Method
tf	634.60	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.09	J/mol×K	1046.18	Joback Method
cpg	1703.75	J/mol×K	1086.36	Joback Method
cpg	1759.46	J/mol×K	1126.54	Joback Method
cpg	1819.89	J/mol×K	1166.72	Joback Method
cpg	1885.66	J/mol×K	1206.90	Joback Method
cpg	1957.44	J/mol×K	1247.07	Joback Method
cpg	2035.86	J/mol×K	1287.25	Joback Method

Sources

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=R110004&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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