cimicifugenol (7-dehydrocycloartenol) acetate

Inchi: InChI=1S/C32H50O2/c1-21(2)10-9-11-22(3)24-14-16-30(8)26-13-12-25-28(5,6)27(34-23
InchiKey: AAOXCALOONADHU-XJVNMOKCSA-N
Formula: C32H50O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCC=C(C)C)=CCC2(C)C4CCC3C1(C)C
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	291.07	kJ/mol	Joback Method
hf	-439.45	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	8.660		Crippen Method
mcvol	406.280	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	3291.00		NIST Webbook
tb	1049.29	K	Joback Method
tc	1293.77	K	Joback Method
tf	687.72	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1641.24	J/mol×K	1049.29	Joback Method
cpg	1703.19	J/mol×K	1090.04	Joback Method
cpg	1771.66	J/mol×K	1130.78	Joback Method
cpg	1847.52	J/mol×K	1171.53	Joback Method
cpg	1931.64	J/mol×K	1212.28	Joback Method
cpg	2024.88	J/mol×K	1253.03	Joback Method
cpg	2128.13	J/mol×K	1293.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111032&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