Cyclosadol (24-methyl-23-dehydrocycloartanol) acetate

Inchi: InChI=1S/C33H54O2/c1-21(2)22(3)10-11-23(4)25-14-16-31(9)27-13-12-26-29(6,7)28(35-
InchiKey: BBSRNANRWHSVJE-MHXLLFDMSA-N
Formula: C33H54O2
SMILES: CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CC=C(C)C(C)C)CCC2(C)C4CCC3C1(C)C
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	269.01	kJ/mol	Joback Method
hf	-532.02	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	90.56	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.986		Crippen Method
mcvol	424.670	ml/mol	McGowan Method
pc	840.65	kPa	Joback Method
rinpol	3441.00		NIST Webbook
tb	1062.92	K	Joback Method
tc	1308.02	K	Joback Method
tf	666.47	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.51	J/mol×K	1062.92	Joback Method
cpg	1821.79	J/mol×K	1103.77	Joback Method
cpg	1893.67	J/mol×K	1144.62	Joback Method
cpg	1973.05	J/mol×K	1185.47	Joback Method
cpg	2060.80	J/mol×K	1226.32	Joback Method
cpg	2157.79	J/mol×K	1267.17	Joback Method
cpg	2264.92	J/mol×K	1308.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111116&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