3,4-dihydro-3-oxoactinidol (isomeric form)

Inchi: InChI=1S/C13H20O3/c1-8(14)10-5-11-12(2,3)6-9(15)7-13(11,4)16-10/h5,8,10,14H,6-7H2
InchiKey: GQMVJMPTJNNDRV-RHYVWVDMSA-N
Formula: C13H20O3
SMILES: CC(O)C1C=C2C(C)(C)CC(=O)CC2(C)O1
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
gf	-202.55	kJ/mol	Joback Method
hf	-555.29	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.840		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
ripol	2456.00		NIST Webbook
ripol	2466.00		NIST Webbook
ripol	2456.00		NIST Webbook
tb	709.59	K	Joback Method
tc	931.33	K	Joback Method
tf	459.04	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.07	J/mol×K	709.59	Joback Method
cpg	564.84	J/mol×K	746.55	Joback Method
cpg	581.20	J/mol×K	783.50	Joback Method
cpg	597.35	J/mol×K	820.46	Joback Method
cpg	613.50	J/mol×K	857.42	Joback Method
cpg	629.87	J/mol×K	894.37	Joback Method
cpg	646.65	J/mol×K	931.33	Joback Method

Sources

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=R335916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume