3,4-dihydro-3-oxoactinidol

Inchi: InChI=1S/C13H22O3/c1-8(14)10-9(15)11-12(2,3)6-5-7-13(11,4)16-10/h8,10-11,14H,5-7H
InchiKey: WELWHPPZYFUSEF-KFLNTJEPSA-N
Formula: C13H22O3
SMILES: CC(O)C1OC2(C)CCCC(C)(C)C2C1=O
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-230.59	kJ/mol	Joback Method
hf	-621.94	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.920		Crippen Method
mcvol	185.620	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	700.78	K	Joback Method
tc	919.94	K	Joback Method
tf	441.52	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.67	J/mol×K	700.78	Joback Method
cpg	593.93	J/mol×K	737.31	Joback Method
cpg	611.62	J/mol×K	773.83	Joback Method
cpg	628.94	J/mol×K	810.36	Joback Method
cpg	646.09	J/mol×K	846.89	Joback Method
cpg	663.28	J/mol×K	883.41	Joback Method

cpg	680.70	J/mol×K	919.94	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=R225215&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume