3,4-dihydro-3-hydroxyactinidol I

Inchi: InChI=1S/C13H22O3/c1-8(14)10-5-11-12(2,3)6-9(15)7-13(11,4)16-10/h5,8-10,14-15H,6-
InchiKey: JZZFHGHGUGITAS-HWMWNZGHSA-N
Formula: C13H22O3
SMILES: CC(O)C1C=C2C(C)(C)CC(O)CC2(C)O1
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-224.49	kJ/mol	Joback Method
hf	-590.16	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.632		Crippen Method
mcvol	185.620	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
ripol	2713.00		NIST Webbook
ripol	2713.00		NIST Webbook
tb	729.28	K	Joback Method
tc	928.20	K	Joback Method
tf	447.40	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.29	J/mol×K	729.28	Joback Method
cpg	595.37	J/mol×K	762.43	Joback Method
cpg	610.18	J/mol×K	795.59	Joback Method
cpg	624.89	J/mol×K	828.74	Joback Method
cpg	639.68	J/mol×K	861.90	Joback Method
cpg	654.71	J/mol×K	895.05	Joback Method
cpg	670.16	J/mol×K	928.20	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=R332853&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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