3-oxo-3,4-dihydro-actinidiolide

Inchi: InChI=1S/C11H14O3/c1-10(2)5-7(12)6-11(3)8(10)4-9(13)14-11/h4H,5-6H2,1-3H3/t11-/m
InchiKey: DJSMGUVSIWKZJW-NSHDSACASA-N
Formula: C11H14O3
SMILES: CC1(C)CC(=O)CC2(C)OC(=O)C=C12
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-195.01	kJ/mol	Joback Method
hf	-473.86	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.617		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
ripol	2681.00		NIST Webbook
ripol	2681.00		NIST Webbook
tb	644.58	K	Joback Method
tc	904.46	K	Joback Method
tf	463.14	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.98	J/mol×K	644.58	Joback Method
cpg	429.19	J/mol×K	687.89	Joback Method
cpg	445.72	J/mol×K	731.21	Joback Method
cpg	461.83	J/mol×K	774.52	Joback Method
cpg	477.80	J/mol×K	817.83	Joback Method
cpg	493.91	J/mol×K	861.14	Joback Method
cpg	510.43	J/mol×K	904.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329807&Units=SI

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