Actinidole

Inchi: InChI=1S/C12H18O2/c1-8(13)11-7-9-10(14-11)5-4-6-12(9,2)3/h4-5,7-8,10-11,13H,6H2,1
InchiKey: SUABBKPMOURIHF-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC(O)C1C=C2C(C=CCC2(C)C)O1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-52.93	kJ/mol	Joback Method
hf	-354.41	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.047		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
ripol	1952.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1952.00		NIST Webbook
tb	617.81	K	Joback Method
tc	826.00	K	Joback Method
tf	356.41	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.20	J/mol×K	617.81	Joback Method
cpg	461.85	J/mol×K	652.51	Joback Method
cpg	476.60	J/mol×K	687.21	Joback Method
cpg	490.60	J/mol×K	721.91	Joback Method
cpg	503.97	J/mol×K	756.60	Joback Method
cpg	516.82	J/mol×K	791.30	Joback Method
cpg	529.28	J/mol×K	826.00	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=R423286&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