trans-actinidol

Inchi: InChI=1S/C13H22O2/c1-9(14)10-8-11-12(2,3)6-5-7-13(11,4)15-10/h8-10,14H,5-7H2,1-4H
InchiKey: NAYQQVFNOVWFLP-UXSKAQMCSA-N
Formula: C13H22O2
SMILES: CC(O)C1C=C2C(C)(C)CCCC2(C)O1
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-79.96	kJ/mol	Joback Method
hf	-417.59	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.661		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	641.77	K	Joback Method
tc	852.34	K	Joback Method
tf	390.82	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.48	J/mol×K	641.77	Joback Method
cpg	533.45	J/mol×K	676.87	Joback Method
cpg	549.65	J/mol×K	711.96	Joback Method
cpg	565.31	J/mol×K	747.06	Joback Method
cpg	580.61	J/mol×K	782.15	Joback Method
cpg	595.78	J/mol×K	817.25	Joback Method
cpg	611.01	J/mol×K	852.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R217308&Units=SI
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

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