1-endo-Boubonanol

Inchi: InChI=1S/C14H24O/c1-8(2)9-6-7-14(3)10-4-5-11(15)12(10)13(9)14/h8-13,15H,4-7H2,1-3
InchiKey: AUSFBWXRTAOCCI-TYKLQLBESA-N
Formula: C14H24O
SMILES: CC(C)C1CCC2(C)C3CCC(O)C3C12
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	69.27	kJ/mol	Joback Method
hf	-323.34	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	60.88	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.076		Crippen Method
mcvol	181.410	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1575.00		NIST Webbook
tb	622.18	K	Joback Method
tc	821.87	K	Joback Method
tf	354.84	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.72	J/mol×K	622.18	Joback Method
cpg	565.09	J/mol×K	655.46	Joback Method
cpg	583.39	J/mol×K	688.74	Joback Method
cpg	600.77	J/mol×K	722.03	Joback Method
cpg	617.37	J/mol×K	755.31	Joback Method
cpg	633.33	J/mol×K	788.59	Joback Method
cpg	648.80	J/mol×K	821.87	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=R196459&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume