endo-1-bourbonanone

Other names: endo-1-Norbourbonanone
Inchi: InChI=1S/C14H22O/c1-8(2)9-6-7-14(3)10-4-5-11(15)12(10)13(9)14/h8-10,12-13H,4-7H2
InchiKey: PYUWACLOPFTHBV-YHVDDPLKSA-N
Formula: C14H22O
SMILES: CC(C)C1CCC2(C)C3CCC(=O)C3C12
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	91.21	kJ/mol	Joback Method
hf	-288.47	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	48.76	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.284		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	602.49	K	Joback Method
tc	830.61	K	Joback Method
tf	366.48	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.78	J/mol×K	602.49	Joback Method
cpg	534.11	J/mol×K	640.51	Joback Method
cpg	555.07	J/mol×K	678.53	Joback Method
cpg	574.84	J/mol×K	716.55	Joback Method
cpg	593.60	J/mol×K	754.57	Joback Method
cpg	611.55	J/mol×K	792.59	Joback Method
cpg	628.85	J/mol×K	830.61	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=R340408&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