15-nor-4-Bourbonene

Inchi: InChI=1S/C14H22/c1-9(2)10-7-8-14(3)12-6-4-5-11(12)13(10)14/h5,9-10,12-13H,4,6-8H2
InchiKey: VOVBFCUKWQPMAL-VZZFWQQMSA-N
Formula: C14H22
SMILES: CC(C)C1CCC2(C)C3CCC=C3C12
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	241.84	kJ/mol	Joback Method
hf	-84.12	kJ/mol	Joback Method
hfus	16.40	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.025		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1563.00		NIST Webbook
tb	543.48	K	Joback Method
tc	761.08	K	Joback Method
tf	315.78	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.27	J/mol×K	543.48	Joback Method
cpg	473.04	J/mol×K	579.75	Joback Method
cpg	493.28	J/mol×K	616.01	Joback Method
cpg	512.16	J/mol×K	652.28	Joback Method
cpg	529.90	J/mol×K	688.55	Joback Method
cpg	546.68	J/mol×K	724.82	Joback Method
cpg	562.69	J/mol×K	761.08	Joback Method

Sources

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=R617411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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