

(-)-«beta»-Bourbonene

Other names:

Cyclobuta[1,2:3,4]dicyclopentene,
decahydro-3a-methyl-6-methylene-1-(1-methylethyl)-
«beta»-bourbonene
[[1S-(1«alpha»,3a«alpha»,3b«beta»,6a«beta»,6b«alpha»)]-
Cyclobuta[1,2:3,4]dicyclopentene,
1,2,3,3a,3b,«beta»,4,5,6,6a«beta»,6b«alpha»-decahydro-1«alpha»-isopropyl-3a«alpha»-
Cyclobuta[1,2:3,4]dicyclopentene,
decahydro-3a-methyl-6-methylene-1-(1-methylethyl)-
(1«alpha»,3a«alpha»,3b«beta»,6a«beta»,6b«alpha»)]-Cyclobuta[1,2:3,4]dicyclopentene,
(1S,3aS,3bR,6aS,6bR)-1-Isopropyl-3a-methyl-6-methylenedecahydrocyclobuta[1,2:3,4]di-
«beta»-bourbenene
Cyclobuta[1,2:3,4]dicyclopentene,
decahydro-3a-methyl-6-methylene-1-(1-methylethyl)-, (1S,3aS,3bR,6aS,6bR)-
beta-bourbonene

Inchi: InChI=1S/C15H24/c1-9(2)11-7-8-15(4)12-6-5-10(3)13(12)14(11)15/h9,11-14H,3,5-8H2,1
InchiKey: YIRAHEODQBQONHI-XTLGRWLVS-A
Formula: C15H24
SMILES: C=C1CCC2C1C1C(C(C)C)CCC21C
Mol. weight [g/mol]: 204.35
CAS: 5208-59-3

Physical Properties

Property code	Value	Unit	Source
gf	275.30	kJ/mol	Joback Method
hf	-87.17	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
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ripol	1529.00		NIST Webbook
ripol	1535.00		NIST Webbook
tb	556.71	K	Joback Method
tc	769.30	K	Joback Method
tf	323.21	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.63	J/mol×K	556.71	Joback Method
cpg	524.39	J/mol×K	592.14	Joback Method
cpg	545.67	J/mol×K	627.57	Joback Method
cpg	565.65	J/mol×K	663.00	Joback Method
cpg	584.49	J/mol×K	698.44	Joback Method
cpg	602.37	J/mol×K	733.87	Joback Method
cpg	619.46	J/mol×K	769.30	Joback Method

Sources

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McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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