

1,5-di-epi-«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:	YIRAHEODBQONHI-NIFZNCRKSA-N
Formula:	C15H24
SMILES:	C=C1CCC2C1C1C(C(C)C)CCC21C
Mol. weight [g/mol]:	204.35

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
rinpol	1385.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1399.00		NIST Webbook
tb	556.71	K	Joback Method
tc	769.30	K	Joback Method
tf	323.21	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.63	J/molxK	556.71	Joback Method
cpg	524.39	J/molxK	592.14	Joback Method
cpg	545.67	J/molxK	627.57	Joback Method
cpg	565.65	J/molxK	663.00	Joback Method
cpg	584.49	J/molxK	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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R424001&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
hvac:	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

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