«alpha»-Bourbonene

Inchi: InChI=1S/C15H24/c1-9(2)11-7-8-15(4)12-6-5-10(3)13(12)14(11)15/h5,9,11-14H,6-8H2,1-
InchiKey: FAIMMSRDTUMTQR-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CCC2C1C1C(C(C)C)CCC21C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	242.55	kJ/mol	Joback Method
hf	-125.10	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1529.00		NIST Webbook

ripol	1506.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1515.00		NIST Webbook
tb	561.69	K	Joback Method
tc	775.53	K	Joback Method
tf	322.81	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.35	J/mol×K	561.69	Joback Method
cpg	525.87	J/mol×K	597.33	Joback Method
cpg	546.93	J/mol×K	632.97	Joback Method
cpg	566.70	J/mol×K	668.61	Joback Method
cpg	585.36	J/mol×K	704.25	Joback Method
cpg	603.09	J/mol×K	739.89	Joback Method
cpg	620.07	J/mol×K	775.53	Joback Method

Sources

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=U293019&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume