

Bourbonanol

Inchi:	InChI=1S/C15H26O/c1-9(2)10-5-7-14(3)11-6-8-15(4,16)13(11)12(10)14/h9-13,16H,5-8H2
InchiKey:	HNNQYJPDMHXZMQ-AFYRIXKGSА-N
Formula:	C15H26O
SMILES:	CC(C)C1CCC2(C)C3CCC(C)(O)C3C12
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	72.20	kJ/mol	Joback Method
hf	-328.74	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1520.00		NIST Webbook
ripol	2047.00		NIST Webbook
tb	645.30	K	Joback Method
tc	849.11	K	Joback Method
tf	390.01	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.91	J/molxK	645.30	Joback Method
cpg	616.48	J/molxK	679.27	Joback Method
cpg	635.16	J/molxK	713.24	Joback Method
cpg	653.15	J/molxK	747.21	Joback Method
cpg	670.70	J/molxK	781.17	Joback Method
cpg	688.01	J/molxK	815.14	Joback Method
cpg	705.32	J/molxK	849.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203700&Units=SI
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

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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