1-endo-Bourbonanol

Inchi: InChI=1S/C15H24O/c1-9(2)15(16)8-7-14(4)11-6-5-10(3)12(11)13(14)15/h9,11-13,16H,3,
InchiKey: REMBOHXSSMDHAC-UHFFFAOYSA-N
Formula: C15H24O
SMILES: C=C1CCC2C1C1C2(C)CCC1(O)C(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	132.99	kJ/mol	Joback Method
hf	-224.16	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	62.42	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1574.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	649.13	K	Joback Method
tc	854.53	K	Joback Method
tf	407.93	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.78	J/mol×K	649.13	Joback Method
cpg	589.92	J/mol×K	683.36	Joback Method
cpg	607.25	J/mol×K	717.60	Joback Method
cpg	624.01	J/mol×K	751.83	Joback Method
cpg	640.42	J/mol×K	786.06	Joback Method
cpg	656.72	J/mol×K	820.29	Joback Method

cpg	673.13	J/mol×K	854.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R283355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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