endo-1-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-YXJLRHLOSA-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
hfus	18.09	kJ/mol	Joback Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
rinpol	1515.00		NIST Webbook

Temperature Dependent Properties

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

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R607013&Units=SI

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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices