Bicyclovetivenol

Inchi: InChI=1S/C15H26O/c1-10-6-5-7-11(2)14-9-12(8-13(10)14)15(3,4)16/h11-14,16H,1,5-9H2
InchiKey: VCECLBDDLTXHHP-NTXGFPLRSA-N
Formula: C15H26O
SMILES: C=C1CCCC(C)C2CC(C(C)(C)O)CC12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	52.20	kJ/mol	Joback Method
hf	-349.39	kJ/mol	Joback Method
hfus	20.13	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
ripol	2604.00		NIST Webbook
ripol	2604.00		NIST Webbook
tb	651.93	K	Joback Method
tc	856.02	K	Joback Method
tf	349.05	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.16	J/mol×K	651.93	Joback Method
cpg	622.83	J/mol×K	685.95	Joback Method
cpg	642.24	J/mol×K	719.96	Joback Method
cpg	660.44	J/mol×K	753.98	Joback Method
cpg	677.48	J/mol×K	787.99	Joback Method

cpg	693.44	J/mol×K	822.01	Joback Method
cpg	708.35	J/mol×K	856.02	Joback Method
dvisc	0.0059008	Pa×s	349.05	Joback Method
dvisc	0.0020979	Pa×s	399.53	Joback Method
dvisc	0.0009406	Pa×s	450.01	Joback Method
dvisc	0.0004958	Pa×s	500.49	Joback Method
dvisc	0.0002939	Pa×s	550.97	Joback Method
dvisc	0.0001902	Pa×s	601.45	Joback Method
dvisc	0.0001317	Pa×s	651.93	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=R324451&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
dvisc:	Dynamic viscosity
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

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