Himachalol

Inchi: InChI=1S/C15H26O/c1-11-6-7-12-13(10-11)14(2,3)8-5-9-15(12,4)16/h10,12-13,16H,5-9H
InchiKey: BBAMLNIPVMLTSQ-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC1=CC2C(CC1)C(C)(O)CCCC2(C)C
Mol. weight [g/mol]: 222.37
CAS: 1891-45-8

Physical Properties

Property code	Value	Unit	Source
gf	-6.47	kJ/mol	Joback Method
hf	-354.25	kJ/mol	Joback Method
hfus	14.84	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1657.40		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1657.40		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1647.00		NIST Webbook

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rinpol	1662.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1647.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2246.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2237.00		NIST Webbook
tb	664.89	K	Joback Method
tc	879.55	K	Joback Method
tf	390.51	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.53	J/mol×K	664.89	Joback Method
cpg	616.99	J/mol×K	700.67	Joback Method
cpg	636.59	J/mol×K	736.44	Joback Method
cpg	655.52	J/mol×K	772.22	Joback Method
cpg	673.99	J/mol×K	808.00	Joback Method
cpg	692.21	J/mol×K	843.77	Joback Method
cpg	710.38	J/mol×K	879.55	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1891458&Units=SI

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

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