3-Hydroxyisodavanone

Inchi: InChI=1S/C15H24O3/c1-6-15(5)8-7-14(18-15)11(4)13(17)9-12(16)10(2)3/h6,9-11,14,16H
InchiKey: IWWJFTCNRBRIRH-JJLXFFRJSA-N
Formula: C15H24O3
SMILES: C=CC1(C)CCC(C(C)C(=O)C=C(O)C(C)C)O1
Mol. weight [g/mol]: 252.35

Physical Properties

Property code	Value	Unit	Source
gf	-98.46	kJ/mol	Joback Method
hf	-472.06	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	74.31	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.413		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	726.29	K	Joback Method
tc	928.60	K	Joback Method
tf	375.89	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.49	J/mol×K	726.29	Joback Method
cpg	655.73	J/mol×K	760.01	Joback Method
cpg	671.31	J/mol×K	793.73	Joback Method
cpg	686.35	J/mol×K	827.44	Joback Method
cpg	700.97	J/mol×K	861.16	Joback Method
cpg	715.29	J/mol×K	894.88	Joback Method
cpg	729.44	J/mol×K	928.60	Joback Method

Sources

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=R226649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume