2-Hydroxyisodavanone

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

Physical Properties

Property code	Value	Unit	Source
gf	-103.73	kJ/mol	Joback Method
hf	-487.12	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.642		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1644.00		NIST Webbook
tb	722.06	K	Joback Method
tc	921.15	K	Joback Method
tf	386.65	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.75	J/mol×K	722.06	Joback Method
cpg	658.12	J/mol×K	755.24	Joback Method
cpg	673.83	J/mol×K	788.42	Joback Method
cpg	688.97	J/mol×K	821.61	Joback Method
cpg	703.67	J/mol×K	854.79	Joback Method
cpg	718.04	J/mol×K	887.97	Joback Method
cpg	732.18	J/mol×K	921.15	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=R89516&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
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