1,2-Dehydro-3-hydroxy-isodavanone

Inchi: InChI=1S/C15H22O3/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: AYJCMTOVQWMEDB-JJLXFFRJSA-N
Formula: C15H22O3
SMILES: C=CC1(C)CCC(C(C)C(=O)C=C(O)C(=C)C)O1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-16.73	kJ/mol	Joback Method
hf	-351.14	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.333		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1601.00		NIST Webbook
tb	723.29	K	Joback Method
tc	928.14	K	Joback Method
tf	375.17	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.13	J/mol×K	723.29	Joback Method
cpg	629.75	J/mol×K	757.43	Joback Method
cpg	644.72	J/mol×K	791.57	Joback Method
cpg	659.19	J/mol×K	825.72	Joback Method
cpg	673.29	J/mol×K	859.86	Joback Method
cpg	687.15	J/mol×K	894.00	Joback Method
cpg	700.90	J/mol×K	928.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226629&Units=SI
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

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