1,2-Dehydro-3,4-dihydro-3-hydroxydavanone

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

Physical Properties

Property code	Value	Unit	Source
gf	-90.84	kJ/mol	Joback Method
hf	-463.85	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.642		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1579.00		NIST Webbook
tb	718.81	K	Joback Method
tc	917.65	K	Joback Method
tf	379.21	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.53	J/mol×K	718.81	Joback Method
cpg	654.69	J/mol×K	751.95	Joback Method
cpg	670.17	J/mol×K	785.09	Joback Method
cpg	685.07	J/mol×K	818.23	Joback Method
cpg	699.50	J/mol×K	851.37	Joback Method
cpg	713.59	J/mol×K	884.51	Joback Method
cpg	727.43	J/mol×K	917.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226614&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