Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzop

Other names: Ketone, 7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl methyl
Alloevodionol
1-(7-Hydroxy-5-methoxy-2,2-dimethyl-2H-chromen-8-yl)ethanone

Inchi: InChI=1S/C14H16O4/c1-8(15)12-10(16)7-11(17-4)9-5-6-14(2,3)18-13(9)12/h5-7,16H,1-4

InchiKey: LTDSNAYFLFUPPT-UHFFFAOYSA-N

Formula: C14H16O4

SMILES: COc1cc(O)c(C(C)=O)c2c1C=CC(C)(C)O2

Mol. weight [g/mol]: 248.27

CAS: 484-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-251.02	kJ/mol	Joback Method
hf	-544.62	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.788		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1899.00		NIST Webbook
rinpol	1899.00		NIST Webbook
ripol	2786.00		NIST Webbook
ripol	2786.00		NIST Webbook
tb	755.61	K	Joback Method
tc	993.51	K	Joback Method
tf	561.05	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.49	J/mol×K	755.61	Joback Method
cpg	548.52	J/mol×K	795.26	Joback Method

cpg	562.28	J/mol×K	834.91	Joback Method
cpg	575.95	J/mol×K	874.56	Joback Method
cpg	589.75	J/mol×K	914.21	Joback Method
cpg	603.86	J/mol×K	953.86	Joback Method
cpg	618.50	J/mol×K	993.51	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=C484184&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume