3-hydroxy-7,8-dihydro-«beta»-ionone

Inchi: InChI=1S/C13H24O2/c1-9-5-8-12(15)13(3,4)11(9)7-6-10(2)14/h10,12,14-15H,5-8H2,1-4H
InchiKey: PCHNRWMSYBNCRR-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CC1=C(CCC(C)O)C(C)(C)C(O)CC1
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-195.55	kJ/mol	Joback Method
hf	-537.33	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	78.09	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.645		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
ripol	2571.00		NIST Webbook
ripol	2571.00		NIST Webbook
ripol	2553.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2550.00		NIST Webbook
ripol	2589.00		NIST Webbook
ripol	2553.00		NIST Webbook
ripol	2566.00		NIST Webbook
tb	705.00	K	Joback Method
tc	890.58	K	Joback Method
tf	395.75	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.96	J/mol×K	705.00	Joback Method

cpg	579.59	J/mol×K	735.93	Joback Method
cpg	593.67	J/mol×K	766.86	Joback Method
cpg	607.28	J/mol×K	797.79	Joback Method
cpg	620.49	J/mol×K	828.72	Joback Method
cpg	633.37	J/mol×K	859.65	Joback Method
cpg	645.99	J/mol×K	890.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220874&Units=SI

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