2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2-(3-methyl-1

Other names: 3-Penten-1-one, 1-[1,2-dihydroxy-3-isovaleryl-5-(3-methyl-2-butenyl)-4-oxo-2-cyclopenten-1-yl]-4-methyl-
Isohumulone
trans-Isohumulone
3,4-dihydroxy-5-(3-methylbut-2-enyl)-2-(3-methyl-1-oxobutyl)-4-(4-methyl-1-oxopent-3-en

Inchi: InChI=1S/C21H30O5/c1-12(2)7-9-15-19(24)18(16(22)11-14(5)6)20(25)21(15,26)17(23)1

InchiKey: QARXXMMQVDCYGZ-UHFFFAOYSA-N

Formula: C21H30O5

SMILES: CC(C)=CCC(=O)C1(O)C(O)=C(C(=O)CC(C)C)C(=O)C1CC=C(C)C

Mol. weight [g/mol]: 362.46

CAS: 25522-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-353.18	kJ/mol	Joback Method
hf	-844.29	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	113.54	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.625		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2715.00		NIST Webbook
tb	1067.41	K	Joback Method
tc	1307.58	K	Joback Method
tf	619.43	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.52	J/mol×K	1067.41	Joback Method
cpg	1071.12	J/mol×K	1107.44	Joback Method
cpg	1092.01	J/mol×K	1147.47	Joback Method
cpg	1113.39	J/mol×K	1187.50	Joback Method

cpg	1135.45	J/mol×K	1227.53	Joback Method
cpg	1158.36	J/mol×K	1267.56	Joback Method
cpg	1182.33	J/mol×K	1307.58	Joback Method

Sources

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=C25522967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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