Gibberellic acid

Other names:

(+)-Gibberillic acid

(1«alpha»,2«beta»,4a«alpha»,4b«beta»,10«beta»)-2,4a,7-Trihydroxy-1-methyl-8-methylg
acid 1,4a-lactone

(1Â«alphaÂ»,2Â«betaÂ»,4aÂ«alphaÂ»,4bÂ«betaÂ»,10Â«betaÂ»)-2,4a,7-Trihydroxy-1-m
acid 1,4a-lactone

(3S,3aS,4S,4aS,6S,8aR,8bR,11S)-6,11-dihydroxy-3-methyl-12-methylene-2-oxo-4a,6-eth

2,4a,7-Trihydroxy-1-methyl-8-methylenegibb-3-ene-1,10-dicarboxylic acid,
acid

1,4a-lactone, (1«alpha»,2«beta»,4a«alpha»,4b«beta»,10«beta»)-

2;4a,7-Trihydroxy-1-methyl-8-methylenegibb-3-ene-1,10-dicarboxylic acid,

1,4a-lactone, (1Â«alphaÂ»,2Â«betaÂ»,4aÂ«alphaÂ»,4bÂ«betaÂ»,10Â«betaÂ»)-

4a,1-(Epoxymethano)-7,9a-methanobenz[a]azulene, gibb-3-ene-1,10-dicarboxylic
acid deriv.

Activol

Berelex

Brellin

Cekugib

GA

GA3

Gib-Sol

Gib-Tabs

Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-,

1,4a-lactone, (1«alpha»,2«beta»,4a«alpha»,4b«beta»,10«beta»)-

Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-,

1,4a-lactone, (1Â«alphaÂ»,2Â«betaÂ»,4aÂ«alphaÂ»,4bÂ«betaÂ»,10Â«betaÂ»)-

Gibb-tabs

Gibberellic acid GA3

Gibberellin

Gibberellin A3

Gibberellin X

Gibberillic acid

Gibrescol

Gibreskol

Grocel

NCI-C55823

NSC 14190

Pro-Gibb

Pro-Gibb Plus

Regulex

Ryzup

Inchi: InChI=1S/C19H22O6/c1-9-7-17-8-18(9,24)5-3-10(17)19-6-4-11(20)16(2,15(23)25-19)13(

InchiKey: IXORZMNAPKEEDV-UHFFFAOYSA-N

Formula: C19H22O6

SMILES: C=C1CC23CC1(O)CCC2C12C=CC(O)C(C)(C(=O)O1)C2C3C(=O)O

Mol. weight [g/mol]: 346.37

CAS: 77-06-5

Physical Properties

Property code	Value	Unit	Source
gf	-321.49	kJ/mol	Joback Method
hf	-780.82	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	118.26	kJ/mol	Joback Method
log10ws	-1.84		Aqueous Solubility Prediction Method
logp	1.027		Crippen Method
mcvol	242.290	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	1086.81	K	Joback Method
tc	1331.37	K	Joback Method
tf	811.05	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.81	J/mol×K	1086.81	Joback Method
cpg	1086.39	J/mol×K	1127.57	Joback Method
cpg	1141.06	J/mol×K	1168.33	Joback Method
cpg	1202.48	J/mol×K	1209.09	Joback Method
cpg	1271.31	J/mol×K	1249.85	Joback Method
cpg	1348.22	J/mol×K	1290.61	Joback Method
cpg	1433.87	J/mol×K	1331.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77065&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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