Gibbane-1,10-dicarboxylic acid, 4a-hydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1«alpha»,4a«alpha»,4b«beta»,10«beta»)-

Other names:	4a«alpha»,4b«beta»-Gibbane-1«alpha»,10«beta»-dicarboxylic acid, 4a-hydroxy-1-methyl-8-methylene-, 1,4a-lactone, methyl ester Gibberellin A9 methyl ester GA9 ester GA9, methyl ester Gibberelline GA9, methyl ester
Inchi:	InChI=1S/C20H26O4/c1-11-9-19-10-12(11)5-6-13(19)20-8-4-7-18(2,17(22)24-20)15(20)1
InchiKey:	GKRMJALKMNRHGF-UHFFFAOYSA-N
Formula:	C20H26O4
SMILES:	C=C1CC23CC1CCC2C12CCCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]:	330.42
CAS:	2112-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-24.37	kJ/mol	Joback Method
hf	-529.67	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.254		Crippen Method
mcvol	248.940	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2322.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2339.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2352.00		NIST Webbook
rinpol	2321.00		NIST Webbook
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
rinpol	2312.00		NIST Webbook

rinpol	2313.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
rinpol	2309.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2332.00		NIST Webbook
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
rinpol	2346.00		NIST Webbook
rinpol	2349.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2321.00		NIST Webbook
rinpol	2332.00		NIST Webbook
rinpol	2309.00		NIST Webbook
rinpol	2332.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	860.84	K	Joback Method
tc	1110.66	K	Joback Method
tf	641.67	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.72	J/mol×K	860.84	Joback Method
cpg	912.88	J/mol×K	902.48	Joback Method
cpg	941.45	J/mol×K	944.11	Joback Method
cpg	971.97	J/mol×K	985.75	Joback Method
cpg	1005.00	J/mol×K	1027.39	Joback Method
cpg	1041.11	J/mol×K	1069.03	Joback Method
cpg	1080.84	J/mol×K	1110.66	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=C2112085&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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