

[2H2]Gibberellin A9-Me

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-RKWHRFJJSA-N
Formula: C20H26O4
SMILES: C=C1CC23CC1CCC2C12CCCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 330.42

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	2302.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2321.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2312.00		NIST Webbook
rinpol	2341.00		NIST Webbook
rinpol	2367.00		NIST Webbook
rinpol	2321.00		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:	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=R180553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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