2,3-Didehydro GA9, Me

Other names: 1,2-didehydro GA9, Me
Inchi: InChI=1S/C20H24O4/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: QDGNFHLTCPXSCV-RKWHRFJJSA-N
Formula: C20H24O4
SMILES: C=C1CC23CC1CCC2C12C=CCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
gf	5.59	kJ/mol	Joback Method
hf	-471.89	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.030		Crippen Method
mcvol	244.640	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2371.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	860.00	K	Joback Method
tc	1111.71	K	Joback Method
tf	642.43	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.88	J/mol×K	860.00	Joback Method
cpg	883.23	J/mol×K	901.95	Joback Method
cpg	911.08	J/mol×K	943.90	Joback Method

cpg	941.00	J/mol×K	985.85	Joback Method
cpg	973.57	J/mol×K	1027.81	Joback Method
cpg	1009.34	J/mol×K	1069.76	Joback Method
cpg	1048.91	J/mol×K	1111.71	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=R281057&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