GA1 1,10-ene diacid, MeTMS

Inchi: InChI=1S/C21H28O4/c1-12-10-21-11-13(12)7-8-15(21)14-6-5-9-20(2,19(23)25-4)16(14)1
InchiKey: WXEWPXFNVFSVOA-LDNWYAMUSA-N
Formula: C21H28O4
SMILES: C=C1CC23CC1CCC2C1=CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-88.19	kJ/mol	Joback Method
hf	-573.30	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	79.01	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.667		Crippen Method
mcvol	269.590	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	866.67	K	Joback Method
tc	1097.77	K	Joback Method
tf	598.23	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.33	J/mol×K	866.67	Joback Method
cpg	944.66	J/mol×K	905.19	Joback Method
cpg	968.23	J/mol×K	943.70	Joback Method
cpg	992.37	J/mol×K	982.22	Joback Method
cpg	1017.38	J/mol×K	1020.74	Joback Method
cpg	1043.57	J/mol×K	1059.25	Joback Method
cpg	1071.26	J/mol×K	1097.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R299360&Units=SI
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

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