GA12 aldehyde, Me-TMS

Inchi: InChI=1S/C21H30O3/c1-13-10-21-11-14(13)6-7-15(21)20(3)9-5-8-19(2,12-22)17(20)16(2
InchiKey: LODKRMFZGMWBOF-KBWCDIBOSA-N
Formula: C21H30O3
SMILES: C=C1CC23CC1CCC2C1(C)CCCC(C)(C=O)C1C3C(=O)OC
Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	12.68	kJ/mol	Joback Method
hf	-465.49	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	74.16	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.163		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	830.47	K	Joback Method
tc	1064.00	K	Joback Method
tf	574.45	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.64	J/mol×K	830.47	Joback Method
cpg	941.40	J/mol×K	869.39	Joback Method
cpg	967.84	J/mol×K	908.31	Joback Method
cpg	995.41	J/mol×K	947.24	Joback Method
cpg	1024.55	J/mol×K	986.16	Joback Method
cpg	1055.71	J/mol×K	1025.08	Joback Method
cpg	1089.34	J/mol×K	1064.00	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=R559152&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