Kaurenic acid, Me-TMS

Inchi: InChI=1S/C21H32O2/c1-14-12-21-11-8-16-19(2,17(21)7-6-15(14)13-21)9-5-10-20(16,3)1
InchiKey: DWTRNJFPDXIFSY-JLDNAQLLSA-N
Formula: C21H32O2
SMILES: C=C1CC23CCC4C(C)(C(=O)OC)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	107.81	kJ/mol	Joback Method
hf	-365.73	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.128		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook
tb	790.75	K	Joback Method
tc	1029.43	K	Joback Method
tf	533.17	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.86	J/mol×K	790.75	Joback Method
cpg	917.63	J/mol×K	830.53	Joback Method
cpg	944.60	J/mol×K	870.31	Joback Method
cpg	972.25	J/mol×K	910.09	Joback Method
cpg	1001.05	J/mol×K	949.87	Joback Method
cpg	1031.48	J/mol×K	989.65	Joback Method
cpg	1064.01	J/mol×K	1029.43	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=R547030&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