ent-Kaurenoic acid, 16,17-dlhydro, 7«alpha», 16«beta»,17-triol, Me

Inchi: InChI=1S/C21H34O5/c1-18-7-4-8-19(2,17(24)26-3)15(18)9-16(23)20-10-13(5-6-14(18)20
InchiKey: PSHLENOGNSMWIY-CAOQSYSXSA-N
Formula: C21H34O5
SMILES: COC(=O)C1(C)CCCC2(C)C1CC(O)C13CC(CCC21)C(O)(CO)C3
Mol. weight [g/mol]: 366.49

Physical Properties

Property code	Value	Unit	Source
gf	-376.64	kJ/mol	Joback Method
hf	-932.10	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	116.03	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.266		Crippen Method
mcvol	288.360	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	1059.03	K	Joback Method
tc	1296.55	K	Joback Method
tf	717.37	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1208.26	J/mol×K	1059.03	Joback Method
cpg	1253.33	J/mol×K	1098.62	Joback Method
cpg	1302.99	J/mol×K	1138.20	Joback Method
cpg	1357.80	J/mol×K	1177.79	Joback Method
cpg	1418.36	J/mol×K	1217.38	Joback Method
cpg	1485.24	J/mol×K	1256.97	Joback Method
cpg	1559.02	J/mol×K	1296.55	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=R490721&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