Methyl-Labd-7-enoate

Inchi: InChI=1S/C21H36O2/c1-15(14-19(22)23-6)8-10-17-16(2)9-11-18-20(3,4)12-7-13-21(17,1
InchiKey: XXMMZZWGGUXLOO-UVLXHGEXSA-N
Formula: C21H36O2
SMILES: COC(=O)CC(C)CCC1C(C)C=CC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
gf	-41.47	kJ/mol	Joback Method
hf	-578.65	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	68.69	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.620		Crippen Method
mcvol	288.170	ml/mol	McGowan Method
pc	1281.91	kPa	Joback Method
rinpol	2218.00		NIST Webbook
tb	771.92	K	Joback Method
tc	983.45	K	Joback Method
tf	441.23	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.77	J/mol×K	771.92	Joback Method
cpg	953.28	J/mol×K	807.18	Joback Method
cpg	977.11	J/mol×K	842.43	Joback Method
cpg	1000.47	J/mol×K	877.69	Joback Method
cpg	1023.57	J/mol×K	912.94	Joback Method
cpg	1046.59	J/mol×K	948.20	Joback Method
cpg	1069.75	J/mol×K	983.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229346&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