Methyl-Labd-8-enoate

Inchi: InChI=1S/C21H34O2/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: JKCGVAHUMWNNIL-ZYKWQNGHSA-N
Formula: C21H34O2
SMILES: COC(=O)CC(C)CCC1=C(C)C=CC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	-15.35	kJ/mol	Joback Method
hf	-503.13	kJ/mol	Joback Method
hfus	27.42	kJ/mol	Joback Method
hvap	70.92	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.685		Crippen Method
mcvol	283.870	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2245.00		NIST Webbook
tb	790.38	K	Joback Method
tc	1005.07	K	Joback Method
tf	475.51	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.59	J/mol×K	790.38	Joback Method
cpg	920.55	J/mol×K	826.16	Joback Method
cpg	943.09	J/mol×K	861.94	Joback Method
cpg	965.42	J/mol×K	897.73	Joback Method
cpg	987.76	J/mol×K	933.51	Joback Method
cpg	1010.32	J/mol×K	969.29	Joback Method
cpg	1033.32	J/mol×K	1005.07	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=R229366&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