Methyl-Labd-8(17)-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: QVGBOMRZGFYUNM-IFXFZGMBSA-N
Formula: C21H34O2
SMILES: C=C1C=CC2C(C)(C)CCCC2(C)C1CCC(C)CC(=O)OC
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	19.32	kJ/mol	Joback Method
hf	-474.07	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	69.15	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.541		Crippen Method
mcvol	283.870	ml/mol	McGowan Method
pc	1331.01	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	775.75	K	Joback Method
tc	988.65	K	Joback Method
tf	459.15	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.06	J/mol×K	775.75	Joback Method
cpg	922.43	J/mol×K	811.23	Joback Method
cpg	945.23	J/mol×K	846.72	Joback Method
cpg	967.67	J/mol×K	882.20	Joback Method
cpg	989.95	J/mol×K	917.68	Joback Method
cpg	1012.27	J/mol×K	953.16	Joback Method
cpg	1034.84	J/mol×K	988.65	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=R229351&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