8-«alpha»-epi-Labdan-14-ene, 13-oxy

Inchi: InChI=1S/C21H38O/c1-7-18(22)16(3)14-15(2)17-10-8-11-19-20(4,5)12-9-13-21(17,19)6/
InchiKey: ZYSCOHWCFLNXKG-YJSIVGGZSA-N
Formula: C21H38O
SMILES: C=CC(O)C(C)CC(C)C1CCCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 306.53

Physical Properties

Property code	Value	Unit	Source
gf	116.34	kJ/mol	Joback Method
hf	-408.65	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.828		Crippen Method
mcvol	286.600	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
ripol	2396.00		NIST Webbook
tb	789.12	K	Joback Method
tc	994.53	K	Joback Method
tf	401.61	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.27	J/mol×K	789.12	Joback Method
cpg	969.97	J/mol×K	823.36	Joback Method
cpg	993.17	J/mol×K	857.59	Joback Method
cpg	1016.09	J/mol×K	891.83	Joback Method
cpg	1038.94	J/mol×K	926.06	Joback Method
cpg	1061.94	J/mol×K	960.30	Joback Method
cpg	1085.30	J/mol×K	994.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410507&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume