(13E)-Labden-8,15-diol

Other names: vulgarol A
Inchi: InChI=1S/C20H36O2/c1-15(10-14-21)7-8-17-19(4)12-6-11-18(2,3)16(19)9-13-20(17,5)22
InchiKey: LEOHDQKUMQKLMP-YHOUDPESSA-N
Formula: C20H36O2
SMILES: CC(=CCO)CCC1C(C)(O)CCC2C(C)(C)CCCC21C
Mol. weight [g/mol]: 308.50
CAS: 10267-31-9

Physical Properties

Property code	Value	Unit	Source
gf	-50.95	kJ/mol	Joback Method
hf	-547.50	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.699		Crippen Method
mcvol	278.380	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
tb	862.67	K	Joback Method
tc	1068.08	K	Joback Method
tf	498.54	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.45	J/mol×K	862.67	Joback Method
cpg	988.51	J/mol×K	896.90	Joback Method
cpg	1013.24	J/mol×K	931.14	Joback Method
cpg	1038.94	J/mol×K	965.37	Joback Method
cpg	1065.88	J/mol×K	999.61	Joback Method
cpg	1094.35	J/mol×K	1033.84	Joback Method

cpg	1124.63	J/mol×K	1068.08	Joback Method

Sources

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=C10267319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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