Labda-8,13-(E)-dien-15-ol

Inchi: InChI=1S/C20H34O/c1-15(11-14-21)7-9-17-16(2)8-10-18-19(3,4)12-6-13-20(17,18)5/h11
InchiKey: IOHVFDUBRDGOCE-UTWTZVNFSA-N
Formula: C20H34O
SMILES: CC(=CCO)CCC1=C(C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	117.48	kJ/mol	Joback Method
hf	-334.99	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.648		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	788.71	K	Joback Method
tc	995.81	K	Joback Method
tf	448.10	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.27	J/mol×K	788.71	Joback Method
cpg	877.92	J/mol×K	823.23	Joback Method
cpg	899.32	J/mol×K	857.74	Joback Method
cpg	920.67	J/mol×K	892.26	Joback Method
cpg	942.21	J/mol×K	926.77	Joback Method
cpg	964.15	J/mol×K	961.29	Joback Method
cpg	986.70	J/mol×K	995.81	Joback Method

Sources

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=R432329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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