15-nor-Labd-8(17)-ene

Inchi: InChI=1S/C19H32/c1-14(2)8-10-16-15(3)9-11-17-18(4,5)12-7-13-19(16,17)6/h16-17H,1,3
InchiKey: XEIZSSHACMVIRI-HHBDYARMSA-N
Formula: C19H32
SMILES: C=C(C)CCC1C(=C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 260.46

Physical Properties

Property code	Value	Unit	Source
gf	288.17	kJ/mol	Joback Method
hf	-124.85	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	6.142		Crippen Method
mcvol	248.250	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1799.00		NIST Webbook
ripol	1971.00		NIST Webbook
tb	651.54	K	Joback Method
tc	867.78	K	Joback Method
tf	362.97	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.85	J/mol×K	651.54	Joback Method
cpg	741.79	J/mol×K	687.58	Joback Method
cpg	765.55	J/mol×K	723.62	Joback Method
cpg	788.37	J/mol×K	759.66	Joback Method
cpg	810.47	J/mol×K	795.70	Joback Method
cpg	832.09	J/mol×K	831.74	Joback Method
cpg	853.45	J/mol×K	867.78	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=R228729&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume