15-nor-Labd-7-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/h9,16-17H,1
InchiKey: FFUKIXRGDHFRHN-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	255.42	kJ/mol	Joback Method
hf	-162.78	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	6.142		Crippen Method
mcvol	248.250	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1835.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2023.00		NIST Webbook
tb	656.52	K	Joback Method
tc	873.82	K	Joback Method
tf	362.57	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.42	J/mol×K	656.52	Joback Method
cpg	743.17	J/mol×K	692.74	Joback Method
cpg	766.78	J/mol×K	728.95	Joback Method
cpg	789.48	J/mol×K	765.17	Joback Method
cpg	811.52	J/mol×K	801.39	Joback Method

cpg	833.12	J/mol×K	837.60	Joback Method
cpg	854.53	J/mol×K	873.82	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=R228714&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume