15-nor-Labd-8-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/h17H,1,7-13
InchiKey: QXUFOBMHYDIQKR-NNBQYGFHSA-N
Formula: C19H32
SMILES: C=C(C)CCC1=C(C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 260.46

Physical Properties

Property code	Value	Unit	Source
gf	253.50	kJ/mol	Joback Method
hf	-153.91	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	56.82	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	6.286		Crippen Method
mcvol	248.250	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1807.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	666.17	K	Joback Method
tc	884.33	K	Joback Method
tf	379.33	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.66	J/mol×K	666.17	Joback Method
cpg	741.73	J/mol×K	702.53	Joback Method
cpg	764.75	J/mol×K	738.89	Joback Method
cpg	786.98	J/mol×K	775.25	Joback Method
cpg	808.66	J/mol×K	811.61	Joback Method
cpg	830.02	J/mol×K	847.97	Joback Method

cpg	851.31	J/mol×K	884.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228734&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
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