Pimara-9(11),5-diene

Inchi: InChI=1S/C20H32/c1-6-19(4)13-10-16-15(14-19)8-9-17-18(2,3)11-7-12-20(16,17)5/h9-10
InchiKey: AOTWRLFKPQTVQG-OAAAQFAESA-N
Formula: C20H32
SMILES: CCC1(C)CC=C2C(CC=C3C(C)(C)CCCC23C)C1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	255.75	kJ/mol	Joback Method
hf	-150.53	kJ/mol	Joback Method
hfus	15.30	kJ/mol	Joback Method
hvap	58.86	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	702.90	K	Joback Method
tc	940.36	K	Joback Method
tf	445.40	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.56	J/mol×K	702.90	Joback Method
cpg	787.30	J/mol×K	742.48	Joback Method
cpg	812.41	J/mol×K	782.05	Joback Method
cpg	837.32	J/mol×K	821.63	Joback Method
cpg	862.48	J/mol×K	861.21	Joback Method
cpg	888.35	J/mol×K	900.78	Joback Method
cpg	915.36	J/mol×K	940.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R302020&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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