19-Norisopimarane

Inchi: InChI=1S/C19H32/c1-5-18(3)12-10-17-15(13-18)8-9-16-14(2)7-6-11-19(16,17)4/h5,14-17
InchiKey: XMQGIJIMPHJDBT-WBWLENEPSA-N
Formula: C19H32
SMILES: C=CC1(C)CCC2C(CCC3C(C)CCCC32C)C1
Mol. weight [g/mol]: 260.46

Physical Properties

Property code	Value	Unit	Source
gf	284.58	kJ/mol	Joback Method
hf	-153.00	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	54.59	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.831		Crippen Method
mcvol	241.690	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	1936.00		NIST Webbook
tb	658.84	K	Joback Method
tc	891.44	K	Joback Method
tf	373.43	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.18	J/mol×K	658.84	Joback Method
cpg	760.39	J/mol×K	697.61	Joback Method
cpg	787.11	J/mol×K	736.37	Joback Method
cpg	812.66	J/mol×K	775.14	Joback Method
cpg	837.36	J/mol×K	813.90	Joback Method
cpg	861.51	J/mol×K	852.67	Joback Method
cpg	885.42	J/mol×K	891.44	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=R548593&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume