Isopimarinal

Inchi: InChI=1S/C20H30O/c1-5-18(2)12-9-16-15(13-18)7-8-17-19(3,14-21)10-6-11-20(16,17)4/
InchiKey: NLLZQKHFTCHPED-GIVJDJEMSA-N
Formula: C20H30O
SMILES: C=CC1(C)CCC2C(=CCC3C(C)(C=O)CCCC23C)C1
Mol. weight [g/mol]: 286.45

Physical Properties

Property code	Value	Unit	Source
gf	216.03	kJ/mol	Joback Method
hf	-177.33	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.321		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2204.00		NIST Webbook
ripol	2854.00		NIST Webbook
ripol	2845.00		NIST Webbook
tb	739.43	K	Joback Method
tc	979.37	K	Joback Method
tf	468.12	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.90	J/mol×K	739.43	Joback Method
cpg	816.13	J/mol×K	779.42	Joback Method
cpg	841.06	J/mol×K	819.41	Joback Method
cpg	866.16	J/mol×K	859.40	Joback Method
cpg	891.89	J/mol×K	899.39	Joback Method
cpg	918.71	J/mol×K	939.38	Joback Method

cpg	947.09	J/mol×K	979.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R167194&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume