8-«beta»-Hydroxyisopimarene

Inchi: InChI=1S/C20H34O/c1-6-18(4)12-8-16-19(5)11-7-10-17(2,3)15(19)9-13-20(16,21)14-18/
InchiKey: IYDAPILQPCDHTO-BLXWGWSPSA-N
Formula: C20H34O
SMILES: C=CC1(C)CCC2C(O)(CCC3C(C)(C)CCCC32C)C1
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	145.20	kJ/mol	Joback Method
hf	-295.39	kJ/mol	Joback Method
hfus	12.29	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.336		Crippen Method
mcvol	261.650	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2103.00		NIST Webbook
tb	774.38	K	Joback Method
tc	1000.33	K	Joback Method
tf	493.32	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.79	J/mol×K	774.38	Joback Method
cpg	891.86	J/mol×K	812.04	Joback Method
cpg	918.41	J/mol×K	849.70	Joback Method
cpg	945.91	J/mol×K	887.36	Joback Method
cpg	974.86	J/mol×K	925.01	Joback Method
cpg	1005.73	J/mol×K	962.67	Joback Method
cpg	1039.02	J/mol×K	1000.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R77315&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