13-epi-Dolabradiene

Inchi: InChI=1S/C20H32/c1-6-18(3)12-13-20(5)16(14-18)10-11-19(4)15(2)8-7-9-17(19)20/h6,16
InchiKey: GHYZJFFJSPZRIU-KJPRWFPHSA-N
Formula: C20H32
SMILES: C=CC1(C)CCC2(C)C(CCC3(C)C(=C)CCCC32)C1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	348.30	kJ/mol	Joback Method
hf	-53.82	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	56.13	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.142		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook
tb	685.79	K	Joback Method
tc	924.17	K	Joback Method
tf	426.52	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.33	J/mol×K	685.79	Joback Method
cpg	788.39	J/mol×K	725.52	Joback Method
cpg	814.52	J/mol×K	765.25	Joback Method
cpg	840.16	J/mol×K	804.98	Joback Method
cpg	865.78	J/mol×K	844.71	Joback Method
cpg	891.81	J/mol×K	884.44	Joback Method
cpg	918.72	J/mol×K	924.17	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=R613875&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