epi-Longipenol

Inchi: InChI=1S/C20H32O/c1-12-5-6-16-13(2)7-10-20(16)11-17(21)19(4)9-8-15(12)18(19)14(20
InchiKey: KCFJHDADOWSHBJ-YNQRBKIGSA-N
Formula: C20H32O
SMILES: C=C1C2C3CCC2(C)C(O)CC12CCC(C)C2CCC3C
Mol. weight [g/mol]: 288.47

Physical Properties

Property code	Value	Unit	Source
gf	186.56	kJ/mol	Joback Method
hf	-308.44	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	73.75	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.802		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	774.18	K	Joback Method
tc	991.11	K	Joback Method
tf	478.18	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.71	J/mol×K	774.18	Joback Method
cpg	881.59	J/mol×K	810.34	Joback Method
cpg	905.00	J/mol×K	846.49	Joback Method
cpg	928.18	J/mol×K	882.65	Joback Method
cpg	951.43	J/mol×K	918.80	Joback Method
cpg	975.01	J/mol×K	954.96	Joback Method
cpg	999.20	J/mol×K	991.11	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=R574537&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