ent-Kaurenol

Inchi: InChI=1S/C20H32O/c1-14-11-20-10-7-16-18(2,13-21)8-4-9-19(16,3)17(20)6-5-15(14)12-

InchiKey: TUJQVRFWMWRMIO-FOEMKWDFSA-N

Formula: C20H32O

SMILES: C=C1CC23CCC4C(C)(CO)CCCC4(C)C2CCC1C3

Mol. weight [g/mol]: 288.47

Physical Properties

Property code	Value	Unit	Source
gf	196.49	kJ/mol	Joback Method
hf	-252.52	kJ/mol	Joback Method
hfus	17.87	kJ/mol	Joback Method
hvap	73.22	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.948		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2302.00		NIST Webbook
tb	783.76	K	Joback Method
tc	1007.15	K	Joback Method
tf	510.56	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.93	J/mol×K	783.76	Joback Method
cpg	872.25	J/mol×K	820.99	Joback Method
cpg	896.77	J/mol×K	858.22	Joback Method
cpg	921.91	J/mol×K	895.46	Joback Method
cpg	948.07	J/mol×K	932.69	Joback Method
cpg	975.66	J/mol×K	969.92	Joback Method
cpg	1005.10	J/mol×K	1007.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R79145&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