8«beta»(H)-Labdane

Inchi: InChI=1S/C20H38/c1-7-15(2)9-11-17-16(3)10-12-18-19(4,5)13-8-14-20(17,18)6/h15-18H
InchiKey: LEWJAHURGICVRE-ZTYBHYHHSA-N
Formula: C20H38
SMILES: CCC(C)CCC1C(C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 278.52

Physical Properties

Property code	Value	Unit	Source
gf	154.07	kJ/mol	Joback Method
hf	-370.99	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	57.01	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.691		Crippen Method
mcvol	270.940	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	673.59	K	Joback Method
tc	881.66	K	Joback Method
tf	357.04	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.24	J/mol×K	673.59	Joback Method
cpg	852.22	J/mol×K	708.27	Joback Method
cpg	878.03	J/mol×K	742.95	Joback Method
cpg	902.88	J/mol×K	777.63	Joback Method
cpg	926.97	J/mol×K	812.31	Joback Method
cpg	950.50	J/mol×K	846.99	Joback Method
cpg	973.68	J/mol×K	881.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312468&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