ent-16«alpha»(H)-Kaurane

Inchi: InChI=1S/C20H34/c1-14-12-20-11-8-16-18(2,3)9-5-10-19(16,4)17(20)7-6-15(14)13-20/h1
InchiKey: IVZWRQBQDVHDNG-RQIKFVFESA-N
Formula: C20H34
SMILES: CC1CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 274.48

Physical Properties

Property code	Value	Unit	Source
gf	272.52	kJ/mol	Joback Method
hf	-204.87	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	6.055		Crippen Method
mcvol	249.220	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	1967.00		NIST Webbook
tb	687.75	K	Joback Method
tc	927.70	K	Joback Method
tf	431.82	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.84	J/mol×K	687.75	Joback Method
cpg	823.76	J/mol×K	727.74	Joback Method
cpg	851.66	J/mol×K	767.73	Joback Method
cpg	879.02	J/mol×K	807.73	Joback Method
cpg	906.36	J/mol×K	847.72	Joback Method
cpg	934.18	J/mol×K	887.71	Joback Method
cpg	962.98	J/mol×K	927.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312473&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