17-Norkaur-15-ene, 13-methyl-, (8«beta»,13«beta»)-

Other names: 17-Nor-8«beta»,13«beta»-kaur-15-ene, 13-methyl-
(+)-Beyerene
(+)-Hibaene
(+)-Stachene
ent-Beyer-15-ene
Beyerene
Hibaene, (+)-
Stachen
Stachene
Stachene, (+)-
Stach-15-ene, (+)-
Hibaene

Inchi: InChI=1S/C20H32/c1-17(2)8-5-9-19(4)15(17)7-11-20-13-12-18(3,14-20)10-6-16(19)20/h1

InchiKey: GXMKKDDGINQVBE-UHFFFAOYSA-N

Formula: C20H32

SMILES: CC12C=CC3(CCC4C(C)(C)CCCC4(C)C3CC1)C2

Mol. weight [g/mol]: 272.47

CAS: 3564-54-3

Physical Properties

Property code	Value	Unit	Source
gf	304.70	kJ/mol	Joback Method
hf	-111.51	kJ/mol	Joback Method
hfus	9.87	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.975		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1941.00		NIST Webbook

ripol	2200.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2200.00		NIST Webbook
tb	691.82	K	Joback Method
tc	943.08	K	Joback Method
tf	460.72	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.29	J/mol×K	691.82	Joback Method
cpg	793.16	J/mol×K	733.70	Joback Method
cpg	820.50	J/mol×K	775.57	Joback Method
cpg	848.06	J/mol×K	817.45	Joback Method
cpg	876.55	J/mol×K	859.33	Joback Method
cpg	906.69	J/mol×K	901.20	Joback Method
cpg	939.22	J/mol×K	943.08	Joback Method

Sources

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=C3564543&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume