

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/h
InchiKey:	GXMKKDDGINQVBE-UHFFFAOYSA-N
Formula:	C20H32
SMILES:	CC12C=CC3(CCC4C(C)(C)CCCC4(C)C3CC1)C2
Mol. weight [g/mol]:	272.47
CAS:	2359-73-1

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	1941.00		NIST Webbook
tb	691.82	K	Joback Method
tc	943.08	K	Joback Method
tf	460.72	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.29	J/molxK	691.82	Joback Method
cpg	793.16	J/molxK	733.70	Joback Method
cpg	820.50	J/molxK	775.57	Joback Method
cpg	848.06	J/molxK	817.45	Joback Method
cpg	876.55	J/molxK	859.33	Joback Method
cpg	906.69	J/molxK	901.20	Joback Method
cpg	939.22	J/molxK	943.08	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=C2359731&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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