

Isohibaene

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-WANGQUDJSA-N
Formula: C20H32
SMILES: CC12C=CC3(CCC4C(C)(C)CCCC4(C)C3CC1)C2
Mol. weight [g/mol]: 272.47
CAS: 5975-53-1

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	1926.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1914.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2245.00		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/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5975531&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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