

5,5-Dimethyl-1-vinylbicyclo[2.1.1]hexane

Inchi:	InChI=1S/C10H16/c1-4-10-6-5-8(7-10)9(10,2)3/h4,8H,1,5-7H2,2-3H3
InchiKey:	FVALSVRBUSTXPB-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C=CC12CCC(C1)C2(C)C
Mol. weight [g/mol]:	136.23
CAS:	16626-39-4

Physical Properties

Property code	Value	Unit	Source
gf	223.97	kJ/mol	Joback Method
hf	31.44	kJ/mol	Joback Method
hfus	5.12	kJ/mol	Joback Method
hvap	34.40	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	920.70		NIST Webbook
tb	434.17	K	Joback Method
tc	645.33	K	Joback Method
tf	280.14	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.95	J/mol×K	434.17	Joback Method
cpg	290.89	J/mol×K	469.36	Joback Method
cpg	308.00	J/mol×K	504.56	Joback Method
cpg	323.51	J/mol×K	539.75	Joback Method
cpg	337.67	J/mol×K	574.94	Joback Method
cpg	350.69	J/mol×K	610.14	Joback Method
cpg	362.82	J/mol×K	645.33	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=C16626394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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