1,3,3-Trimethylcyclopropene

Other names: Cyclopropene-1,3,3-trimethyl
Inchi: InChI=1S/C6H10/c1-5-4-6(5,2)3/h4H,1-3H3
InchiKey: MRLAULBRWNYTDV-UHFFFAOYSA-N
Formula: C6H10
SMILES: CC1=CC1(C)C
Mol. weight [g/mol]: 82.14
CAS: 3664-56-0

Physical Properties

Property code	Value	Unit	Source
affp	895.40	kJ/mol	NIST Webbook
basg	865.90	kJ/mol	NIST Webbook
gf	75.23	kJ/mol	Joback Method
hf	-32.82	kJ/mol	Joback Method
hfus	3.97	kJ/mol	Joback Method
hvap	26.80 ± 1.70	kJ/mol	NIST Webbook
hvap	27.90 ± 1.40	kJ/mol	NIST Webbook
ie	8.58 ± 0.05	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.973		Crippen Method
mcvol	80.240	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	347.80	K	Joback Method
tc	538.54	K	Joback Method
tf	212.50	K	Joback Method
vc	0.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.06	J/mol×K	347.80	Joback Method
cpg	144.66	J/mol×K	379.59	Joback Method

cpg	155.30	J/mol×K	411.38	Joback Method
cpg	165.05	J/mol×K	443.17	Joback Method
cpg	174.00	J/mol×K	474.96	Joback Method
cpg	182.24	J/mol×K	506.75	Joback Method
cpg	189.85	J/mol×K	538.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3664560&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

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume