Cyclohexane, (1-methylethylidene)-

Other names: Cyclohexane, isopropylidene-
Isopropylidenecyclohexane
Inchi: InChI=1S/C9H16/c1-8(2)9-6-4-3-5-7-9/h3-7H2,1-2H3
InchiKey: CUYJYVAWBJXBIC-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC(C)=C1CCCCC1
Mol. weight [g/mol]: 124.22
CAS: 5749-72-4

Physical Properties

Property code	Value	Unit	Source
gf	93.97	kJ/mol	Joback Method
hf	-88.19	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	37.23	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	955.30		NIST Webbook
rinpol	960.70		NIST Webbook
tb	434.00 ± 5.00	K	NIST Webbook
tb	435.00 ± 2.00	K	NIST Webbook
tb	433.00 ± 4.00	K	NIST Webbook
tb	437.00 ± 3.00	K	NIST Webbook
tb	434.00 ± 4.00	K	NIST Webbook
tc	647.27	K	Joback Method
tf	199.21	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.39	J/mol×K	436.06	Joback Method

cpg	259.79	J/mol×K	471.26	Joback Method
cpg	276.24	J/mol×K	506.46	Joback Method
cpg	291.79	J/mol×K	541.66	Joback Method
cpg	306.47	J/mol×K	576.86	Joback Method
cpg	320.31	J/mol×K	612.06	Joback Method
cpg	333.35	J/mol×K	647.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5749724&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

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