isopropenylcyclohexane

Other names: Cyclohexane, 1-methylethenyl
Inchi: InChI=1S/C9H16/c1-8(2)9-6-4-3-5-7-9/h9H,1,3-7H2,2H3
InchiKey: SWLGTNLRTUGMHV-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=C(C)C1CCCCC1
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	128.64	kJ/mol	Joback Method
hf	-59.13	kJ/mol	Joback Method
hfus	8.31	kJ/mol	Joback Method
hvap	35.47	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	924.60		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	920.50		NIST Webbook
tb	421.43	K	Joback Method
tc	629.03	K	Joback Method
tf	182.85	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.08	J/mol×K	421.43	Joback Method
cpg	257.45	J/mol×K	456.03	Joback Method
cpg	274.86	J/mol×K	490.63	Joback Method
cpg	291.34	J/mol×K	525.23	Joback Method
cpg	306.93	J/mol×K	559.83	Joback Method

cpg	321.64	J/mol×K	594.43	Joback Method
cpg	335.51	J/mol×K	629.03	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=R15888&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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