1,4-Cyclohexadiene, 1-(1-methylethenyl)

Inchi: InChI=1S/C9H12/c1-8(2)9-6-4-3-5-7-9/h3-4,7H,1,5-6H2,2H3
InchiKey: WXSSKVGGMFMFAA-UHFFFAOYSA-N
Formula: C9H12
SMILES: C=C(C)C1=CCC=CC1
Mol. weight [g/mol]: 120.19

Physical Properties

Property code	Value	Unit	Source
gf	186.64	kJ/mol	Joback Method
hf	65.30	kJ/mol	Joback Method
hfus	9.29	kJ/mol	Joback Method
hvap	37.02	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.839		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	997.00		NIST Webbook
tb	429.40	K	Joback Method
tc	643.37	K	Joback Method
tf	201.13	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.82	J/mol×K	429.40	Joback Method
cpg	227.77	J/mol×K	465.06	Joback Method
cpg	241.85	J/mol×K	500.72	Joback Method
cpg	255.08	J/mol×K	536.38	Joback Method
cpg	267.51	J/mol×K	572.05	Joback Method
cpg	279.18	J/mol×K	607.71	Joback Method
cpg	290.12	J/mol×K	643.37	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=R127196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume