1-Cyclohexyl-1-propyne

Inchi: InChI=1S/C9H14/c1-2-6-9-7-4-3-5-8-9/h9H,3-5,7-8H2,1H3
InchiKey: IWDWSCMNLSLHKQ-UHFFFAOYSA-N
Formula: C9H14
SMILES: CC#CC1CCCCC1
Mol. weight [g/mol]: 122.21
CAS: 18736-95-3

Physical Properties

Property code	Value	Unit	Source
gf	252.15	kJ/mol	Joback Method
hf	97.53	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	38.21	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.590		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	436.00 ± 1.00	K	NIST Webbook
tc	662.36	K	Joback Method
tf	304.67	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.57	J/mol×K	433.87	Joback Method
cpg	246.52	J/mol×K	471.95	Joback Method
cpg	263.49	J/mol×K	510.03	Joback Method
cpg	279.53	J/mol×K	548.11	Joback Method
cpg	294.64	J/mol×K	586.19	Joback Method
cpg	308.87	J/mol×K	624.27	Joback Method
cpg	322.24	J/mol×K	662.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18736953&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

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