Cyclopropane, trans-1,2-diethynyl-

Inchi: InChI=1S/C7H6/c1-3-6-5-7(6)4-2/h1-2,6-7H,5H2/t6-,7-/m0/s1
InchiKey: WFICLMYHCKJIFK-BQBZGAKWSA-N
Formula: C7H6
SMILES: C#CC1CC1C#C
Mol. weight [g/mol]: 90.12
CAS: 35295-57-9

Physical Properties

Property code	Value	Unit	Source
gf	507.24	kJ/mol	Joback Method
hf	448.45	kJ/mol	Joback Method
hfus	19.04	kJ/mol	Joback Method
hvap	30.50	kJ/mol	Joback Method
ie	9.00 ± 0.02	eV	NIST Webbook
log10ws	-1.75		Crippen Method
logp	0.889		Crippen Method
mcvol	81.430	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
tb	341.87	K	Joback Method
tc	547.56	K	Joback Method
tf	276.29	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.91	J/mol×K	341.87	Joback Method
cpg	144.40	J/mol×K	376.15	Joback Method
cpg	154.17	J/mol×K	410.43	Joback Method
cpg	163.25	J/mol×K	444.72	Joback Method
cpg	171.69	J/mol×K	479.00	Joback Method
cpg	179.53	J/mol×K	513.28	Joback Method
cpg	186.81	J/mol×K	547.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35295579&Units=SI

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
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