(Z)-3,5-Hexadien-1-yne

Inchi: InChI=1S/C6H6/c1-3-5-6-4-2/h1,4-6H,2H2/b6-5-
InchiKey: OGWJYLKDZYZYBA-WAYWQWQTSA-N
Formula: C6H6
SMILES: C#CC=CC=C
Mol. weight [g/mol]: 78.11
CAS: 5222-76-4

Physical Properties

Property code	Value	Unit	Source
gf	390.77	kJ/mol	Joback Method
hf	367.38	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	28.10	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.362		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	327.64	K	Joback Method
tc	516.95	K	Joback Method
tf	197.51	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.82	J/mol×K	327.64	Joback Method
cpg	120.78	J/mol×K	359.19	Joback Method
cpg	128.24	J/mol×K	390.74	Joback Method
cpg	135.23	J/mol×K	422.30	Joback Method
cpg	141.78	J/mol×K	453.85	Joback Method
cpg	147.90	J/mol×K	485.40	Joback Method
cpg	153.64	J/mol×K	516.95	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=C5222764&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume