1,5-Hexadien-3-yne, 2,5-dimethyl-

Other names: Hexa-1,5-diene-3-yne, 2,5-dimethyl-
Inchi: InChI=1S/C8H10/c1-7(2)5-6-8(3)4/h1,3H2,2,4H3
InchiKey: QZXJPGFNLZJNAR-UHFFFAOYSA-N
Formula: C8H10
SMILES: C=C(C)C#CC(=C)C
Mol. weight [g/mol]: 106.17
CAS: 3725-05-1

Physical Properties

Property code	Value	Unit	Source
gf	377.86	kJ/mol	Joback Method
hf	295.13	kJ/mol	Joback Method
hfus	14.42	kJ/mol	Joback Method
hvap	34.37	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-2.67		Crippen Method
logp	2.142		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
tb	384.56	K	Joback Method
tc	588.60	K	Joback Method
tf	254.58	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.58	J/mol×K	384.56	Joback Method
cpg	190.67	J/mol×K	418.57	Joback Method
cpg	201.20	J/mol×K	452.57	Joback Method
cpg	211.19	J/mol×K	486.58	Joback Method
cpg	220.66	J/mol×K	520.59	Joback Method

cpg	229.65	J/mol×K	554.59	Joback Method
cpg	238.18	J/mol×K	588.60	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=C3725051&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
ie:	Ionization energy
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