1,2-Hexadiene

Inchi: InChI=1S/C6H10/c1-3-5-6-4-2/h5H,1,4,6H2,2H3
InchiKey: XIAJQOBRHVKGSP-UHFFFAOYSA-N
Formula: C6H10
SMILES: C=C=CCCC
Mol. weight [g/mol]: 82.14
CAS: 592-44-9

Physical Properties

Property code	Value	Unit	Source
gf	215.76	kJ/mol	Joback Method
hf	121.04	kJ/mol	Joback Method
hfus	12.15	kJ/mol	Joback Method
hvap	28.71	kJ/mol	Joback Method
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.128		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	351.00 ± 2.00	K	NIST Webbook
tb	348.65 ± 4.00	K	NIST Webbook
tb	348.00 ± 2.00	K	NIST Webbook
tc	514.92	K	Joback Method
tf	162.13	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.77	J/mol×K	336.63	Joback Method
cpg	148.37	J/mol×K	366.35	Joback Method
cpg	156.69	J/mol×K	396.06	Joback Method
cpg	164.75	J/mol×K	425.78	Joback Method
cpg	172.54	J/mol×K	455.49	Joback Method
cpg	180.07	J/mol×K	485.21	Joback Method

cpg	187.34	J/mol×K	514.92	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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol366.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592449&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