2,3-Hexadiene

Inchi: InChI=1S/C6H10/c1-3-5-6-4-2/h3,6H,4H2,1-2H3
InchiKey: DPUXQWOMYBMHRN-UHFFFAOYSA-N
Formula: C6H10
SMILES: CC=C=CCC
Mol. weight [g/mol]: 82.14
CAS: 592-49-4

Physical Properties

Property code	Value	Unit	Source
gf	208.14	kJ/mol	Joback Method
hf	112.83	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	29.34	kJ/mol	Joback Method
ie	8.76 ± 0.05	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.128		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	341.15 ± 1.00	K	NIST Webbook
tc	528.46	K	Joback Method
tf	158.81	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.55	J/mol×K	344.11	Joback Method
cpg	147.61	J/mol×K	374.83	Joback Method
cpg	156.32	J/mol×K	405.56	Joback Method
cpg	164.71	J/mol×K	436.28	Joback Method
cpg	172.77	J/mol×K	467.01	Joback Method
cpg	180.51	J/mol×K	497.73	Joback Method
cpg	187.95	J/mol×K	528.46	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol372.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592494&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

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