2,3-Hexadiene, 2-methyl-

Other names: 2-methyl-2,3-hexadiene
Inchi: InChI=1S/C7H12/c1-4-5-6-7(2)3/h5H,4H2,1-3H3
InchiKey: LNCOYAGAIDDTKZ-UHFFFAOYSA-N
Formula: C7H12
SMILES: CCC=C=C(C)C
Mol. weight [g/mol]: 96.17
CAS: 29212-09-7

Physical Properties

Property code	Value	Unit	Source
gf	208.01	kJ/mol	Joback Method
hf	82.40	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	31.65	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.518		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
tb	366.87	K	Joback Method
tc	554.61	K	Joback Method
tf	156.12	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.56	J/mol×K	366.87	Joback Method
cpg	183.32	J/mol×K	398.16	Joback Method
cpg	193.66	J/mol×K	429.45	Joback Method
cpg	203.58	J/mol×K	460.74	Joback Method
cpg	213.10	J/mol×K	492.03	Joback Method
cpg	222.23	J/mol×K	523.32	Joback Method
cpg	230.98	J/mol×K	554.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29212097&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
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