2,4-Hexadiene, 3-methyl-

Other names: 3-Methyl-2,4-hexadiene
Inchi: InChI=1S/C7H12/c1-4-6-7(3)5-2/h4-6H,1-3H3/b6-4+,7-5+
InchiKey: KOXWOWPVSGRFCZ-YDFGWWAZSA-N
Formula: C7H12
SMILES: CC=CC(C)=CC
Mol. weight [g/mol]: 96.17
CAS: 28823-42-9

Physical Properties

Property code	Value	Unit	Source
gf	159.95	kJ/mol	Joback Method
hf	36.84	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	31.17	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	381.00 ± 3.00	K	NIST Webbook
tc	553.14	K	Joback Method
tf	144.53	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.25	J/mol×K	367.76	Joback Method
cpg	177.97	J/mol×K	398.66	Joback Method
cpg	189.07	J/mol×K	429.55	Joback Method
cpg	199.58	J/mol×K	460.45	Joback Method
cpg	209.52	J/mol×K	491.34	Joback Method
cpg	218.94	J/mol×K	522.24	Joback Method
cpg	227.85	J/mol×K	553.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28823429&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