2,4-Hexadiene, 2-methyl-

Other names: 2-Methyl-2,4-hexadiene
Inchi: InChI=1S/C7H12/c1-4-5-6-7(2)3/h4-6H,1-3H3/b5-4+
InchiKey: PRTJSZPCEHPORP-SNAWJCMRSA-N
Formula: C7H12
SMILES: CC=CC=C(C)C
Mol. weight [g/mol]: 96.17
CAS: 28823-41-8

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
rinpol	751.00		NIST Webbook
rinpol	706.00		NIST Webbook
tb	384.70 ± 2.00	K	NIST Webbook
tb	380.00 ± 2.00	K	NIST Webbook
tc	553.14	K	Joback Method
tf	198.60 ± 2.00	K	NIST Webbook
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45188e+01
Coeff. B	-3.43167e+03
Coeff. C	-4.80830e+01
Temperature range (K), min.	289.22
Temperature range (K), max.	420.79

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=389

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28823418&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume