2,4-Hexadiene, 2,5-dimethyl-

Other names:	(CH3)2C=CHCH=C(CH3)2
	2,5-Dimethyl-2,4-hexadiene
	2,5-Dimethylhexa-2,4-diene
	BIISOBUTENYL
	BIISOCROTYL
	Diisocrotyl
	NSC 10812
Inchi:	InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h5-6H,1-4H3
InchiKey:	DZPCYXCBXGQBRN-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC(C)=CC=C(C)C
Mol. weight [g/mol]:	110.20
CAS:	764-13-6

Physical Properties

Property code	Value	Unit	Source
chl	-5085.77 ± 0.70	kJ/mol	NIST Webbook
gf	159.82	kJ/mol	Joback Method
hf	-19.20 ± 0.84	kJ/mol	NIST Webbook
hfl	-63.12 ± 0.84	kJ/mol	NIST Webbook
hfus	14.26	kJ/mol	Joback Method
hvap	43.92 ± 0.05	kJ/mol	NIST Webbook
ie	7.67	eV	NIST Webbook
ie	7.65	eV	NIST Webbook
ie	7.91 ± 0.04	eV	NIST Webbook
ie	7.67	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	821.00		NIST Webbook

rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
ripol	1032.00		NIST Webbook
tb	390.52	K	Joback Method
tc	578.76	K	Joback Method
tf	287.09 ± 1.00	K	NIST Webbook
tf	287.90 ± 2.00	K	NIST Webbook
tf	286.81 ± 0.50	K	NIST Webbook
tf	287.10 ± 1.00	K	NIST Webbook
tf	287.05 ± 0.50	K	NIST Webbook
tf	287.10 ± 1.00	K	NIST Webbook
tf	286.81 ± 0.30	K	NIST Webbook
tf	287.10 ± 1.00	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.58	J/mol×K	390.52	Joback Method
cpg	216.76	J/mol×K	421.89	Joback Method
cpg	229.24	J/mol×K	453.27	Joback Method
cpg	241.05	J/mol×K	484.64	Joback Method
cpg	252.25	J/mol×K	516.01	Joback Method
cpg	262.84	J/mol×K	547.39	Joback Method
cpg	272.88	J/mol×K	578.76	Joback Method
cpl	459.00	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57350e+01
Coeff. B	-3.91653e+03
Coeff. C	-5.46880e+01
Temperature range (K), min.	286.80
Temperature range (K), max.	430.43

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.50466e+01
Coeff. B	-8.42143e+03
Coeff. C	-1.18285e+01
Coeff. D	7.84032e-06
Temperature range (K), min.	313.15
Temperature range (K), max.	447.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol394.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C764136&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=394
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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