1,5-Hexadiene, 2,5-dimethyl-

Other names: 2,5-Dimethyl-1,5-hexadiene
2,5-Dimethylhexa-1,5-diene
BIMETHALLYL
CH2=C(CH3)CH2CH2C(CH3)=CH2
DIMETHALLYL
Inchi: InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h1,3,5-6H2,2,4H3
InchiKey: DSAYAFZWRDYBQY-UHFFFAOYSA-N
Formula: C8H14
SMILES: C=C(C)CCC(=C)C
Mol. weight [g/mol]: 110.20
CAS: 627-58-7

Physical Properties

Property code	Value	Unit	Source
gf	175.06	kJ/mol	Joback Method
hf	22.83	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	32.22	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	766.00		NIST Webbook
tb	387.50 ± 0.50	K	NIST Webbook
tb	387.50 ± 1.00	K	NIST Webbook
tb	387.45 ± 0.50	K	NIST Webbook
tb	387.50	K	NIST Webbook
tb	387.60 ± 1.00	K	NIST Webbook
tb	387.50 ± 0.50	K	NIST Webbook
tb	387.45 ± 0.50	K	NIST Webbook
tb	387.45 ± 0.40	K	NIST Webbook
tc	552.67	K	Joback Method
tf	197.55 ± 0.50	K	NIST Webbook
tf	197.55 ± 0.40	K	NIST Webbook

tf	197.60 ± 0.50	K	NIST Webbook
tf	197.55 ± 0.50	K	NIST Webbook
tf	197.60 ± 0.50	K	NIST Webbook
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.96	J/mol×K	523.15	Joback Method
cpg	203.37	J/mol×K	375.56	Joback Method
cpg	215.74	J/mol×K	405.08	Joback Method
cpg	227.57	J/mol×K	434.60	Joback Method
cpg	238.87	J/mol×K	464.12	Joback Method
cpg	249.66	J/mol×K	493.63	Joback Method
cpg	269.79	J/mol×K	552.67	Joback Method
hvapt	38.80	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55590e+01
Coeff. B	-3.70482e+03
Coeff. C	-4.88610e+01
Temperature range (K), min.	291.46
Temperature range (K), max.	410.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.94769e+02
Coeff. B	-2.04373e+04
Coeff. C	-5.79070e+01
Coeff. D	5.10658e-05
Temperature range (K), min.	330.15
Temperature range (K), max.	388.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol393.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627587&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=393
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
hvapt:	Enthalpy of vaporization at a given temperature
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