1,5-hexadiene, 3,3-dimethyl-

Other names: 3,3-Dimethyl-1,5-hexadiene
Inchi: InChI=1S/C8H14/c1-5-7-8(3,4)6-2/h5-6H,1-2,7H2,3-4H3
InchiKey: OWRACTVEYJLPRK-UHFFFAOYSA-N
Formula: C8H14
SMILES: C=CCC(C)(C)C=C
Mol. weight [g/mol]: 110.20
CAS: 24253-25-6

Physical Properties

Property code	Value	Unit	Source
gf	195.00	kJ/mol	Joback Method
hf	33.66	kJ/mol	Joback Method
hfus	6.50	kJ/mol	Joback Method
hvap	30.77	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.775		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
tb	374.80 ± 2.00	K	NIST Webbook
tc	554.27	K	Joback Method
tf	178.82	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.26	J/mol×K	372.57	Joback Method
cpg	217.83	J/mol×K	402.85	Joback Method
cpg	230.66	J/mol×K	433.14	Joback Method
cpg	242.80	J/mol×K	463.42	Joback Method
cpg	254.27	J/mol×K	493.71	Joback Method
cpg	265.10	J/mol×K	523.99	Joback Method
cpg	275.33	J/mol×K	554.27	Joback Method
dvisc	0.0080123	Pa×s	178.82	Joback Method

dvisc	0.0029353	Pa×s	211.11	Joback Method
dvisc	0.0014036	Pa×s	243.40	Joback Method
dvisc	0.0007978	Pa×s	275.69	Joback Method
dvisc	0.0005105	Pa×s	307.99	Joback Method
dvisc	0.0003556	Pa×s	340.28	Joback Method
dvisc	0.0002637	Pa×s	372.57	Joback Method
hvapt	35.20	kJ/mol	332.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.19667e+01
Coeff. B	-3.04739e+03
Temperature range (K), min.	260.93
Temperature range (K), max.	457.89

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24253256&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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume