(Z)-2,5-Dimethylhex-3-ene

Other names: 3-Hexene, 2,5-dimethyl-, (Z)-
(Z)-2,5-Dimethyl-3-hexene
Inchi: InChI=1S/C8H16/c1-7(2)5-6-8(3)4/h5-8H,1-4H3/b6-5-
InchiKey: KNCMKWVOMRUHKZ-WAYWQWQTSA-N
Formula: C8H16
SMILES: CC(C)C=CC(C)C
Mol. weight [g/mol]: 112.21
CAS: 10557-44-5

Physical Properties

Property code	Value	Unit	Source
chl	-5273.80 ± 1.20	kJ/mol	NIST Webbook
chl	-5283.70 ± 1.80	kJ/mol	NIST Webbook
gf	91.82	kJ/mol	Joback Method
hf	-111.30	kJ/mol	NIST Webbook
hfl	-151.10 ± 1.80	kJ/mol	NIST Webbook
hfus	9.63	kJ/mol	Joback Method
hvap	37.20	kJ/mol	NIST Webbook
ie	8.85 ± 0.01	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	696.60		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	683.90		NIST Webbook
tb	371.80 ± 0.70	K	NIST Webbook
tc	565.78	K	Joback Method
tf	144.84	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	217.83	J/mol×K	385.72	Joback Method
cpg	231.54	J/mol×K	415.73	Joback Method
cpg	244.62	J/mol×K	445.74	Joback Method
cpg	257.12	J/mol×K	475.75	Joback Method
cpg	269.06	J/mol×K	505.76	Joback Method
cpg	280.44	J/mol×K	535.77	Joback Method
cpg	291.30	J/mol×K	565.78	Joback Method
dvisc	0.0231611	Pa×s	144.84	Joback Method
dvisc	0.0043531	Pa×s	184.99	Joback Method
dvisc	0.0014851	Pa×s	225.13	Joback Method
dvisc	0.0007016	Pa×s	265.28	Joback Method
dvisc	0.0004036	Pa×s	305.43	Joback Method
dvisc	0.0002641	Pa×s	345.57	Joback Method
dvisc	0.0001887	Pa×s	385.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10557445&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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