

3-Hexene, 2,5-dimethyl-

Other names:	2,5-Dimethyl-3-hexene
Inchi:	InChI=1S/C8H16/c1-7(2)5-6-8(3)4/h5-8H,1-4H3
InchiKey:	KNCMKQVOMRUHKZ-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC(C)C=CC(C)C
Mol. weight [g/mol]:	112.21
CAS:	15910-22-2

Physical Properties

Property code	Value	Unit	Source
gf	91.82	kJ/mol	Joback Method
hf	-101.79	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	32.58	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	374.90 ± 3.00	K	NIST Webbook
tc	565.78	K	Joback Method
tf	144.84	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/mol×K	385.72	Joback Method
cpg	280.44	J/mol×K	535.77	Joback Method
cpg	269.06	J/mol×K	505.76	Joback Method
cpg	257.12	J/mol×K	475.75	Joback Method
cpg	244.62	J/mol×K	445.74	Joback Method
cpg	231.54	J/mol×K	415.73	Joback Method
cpg	291.30	J/mol×K	565.78	Joback Method
dvisc	0.0001887	Paxs	385.72	Joback Method

dvisc	0.0002641	Paxs	345.57	Joback Method
dvisc	0.0004036	Paxs	305.43	Joback Method
dvisc	0.0007016	Paxs	265.28	Joback Method
dvisc	0.0014851	Paxs	225.13	Joback Method
dvisc	0.0043531	Paxs	184.99	Joback Method
dvisc	0.0231611	Paxs	144.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15910222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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