

(Z)-2-Hexene, 4,5-dimethyl

Inchi:	InChI=1S/C9H18/c1-5-7-9(4)8(3)6-2/h5,7-9H,6H2,1-4H3/b7-5-
InchiKey:	HXSUSWIKNRAROU-ALCCZGGFSA-N
Formula:	C9H18
SMILES:	CC=CC(C)C(C)CC
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	100.24	kJ/mol	Joback Method
hf	-122.43	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	34.81	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.245		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	746.00		NIST Webbook
tb	408.60	K	Joback Method
tc	587.67	K	Joback Method
tf	156.11	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.97	J/mol×K	408.60	Joback Method
cpg	272.79	J/mol×K	438.45	Joback Method
cpg	286.94	J/mol×K	468.29	Joback Method
cpg	300.46	J/mol×K	498.14	Joback Method
cpg	313.37	J/mol×K	527.98	Joback Method
cpg	325.70	J/mol×K	557.83	Joback Method
cpg	337.45	J/mol×K	587.67	Joback Method
dvisc	0.0223846	Paxs	156.11	Joback Method
dvisc	0.0043187	Paxs	198.19	Joback Method

dvisc	0.0014827	Paxs	240.27	Joback Method
dvisc	0.0007001	Paxs	282.36	Joback Method
dvisc	0.0004016	Paxs	324.44	Joback Method
dvisc	0.0002618	Paxs	366.52	Joback Method
dvisc	0.0001863	Paxs	408.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R568631&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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

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