

2-Hexene, 4,5-dimethyl-

Other names:	4,5-dimethyl-2-hexene (cis,trans unspecified)
Inchi:	InChI=1S/C8H16/c1-5-6-8(4)7(2)3/h5-8H,1-4H3
InchiKey:	OAVNNZUEVHCKP-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC=CC(C)C(C)C
Mol. weight [g/mol]:	112.21
CAS:	73548-71-7

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
rinpol	736.00		NIST Webbook
tb	382.95 ± 0.50	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	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	Pa×s	385.72	Joback Method
dvisc	0.0002641	Pa×s	345.57	Joback Method
dvisc	0.0004036	Pa×s	305.43	Joback Method
dvisc	0.0007016	Pa×s	265.28	Joback Method
dvisc	0.0014851	Pa×s	225.13	Joback Method
dvisc	0.0043531	Pa×s	184.99	Joback Method
dvisc	0.0231611	Pa×s	144.84	Joback Method

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=C73548717&Units=SI
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
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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