

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

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

Physical Properties

Property code	Value	Unit	Source
gf	107.96	kJ/mol	Joback Method
hf	-120.62	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	34.29	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mvol	133.370	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
tb	406.25	K	Joback Method
tc	588.59	K	Joback Method
tf	188.53	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.57	J/mol×K	406.25	Joback Method
cpg	329.51	J/mol×K	558.20	Joback Method
cpg	317.00	J/mol×K	527.81	Joback Method
cpg	303.79	J/mol×K	497.42	Joback Method
cpg	289.84	J/mol×K	467.03	Joback Method
cpg	275.11	J/mol×K	436.64	Joback Method
cpg	341.36	J/mol×K	588.59	Joback Method
dvisc	0.0002180	Paxs	406.25	Joback Method

dvisc	0.0003038	Paxs	369.96	Joback Method
dvisc	0.0004551	Paxs	333.68	Joback Method
dvisc	0.0007523	Paxs	297.39	Joback Method
dvisc	0.0014301	Paxs	261.10	Joback Method
dvisc	0.0033453	Paxs	224.82	Joback Method
dvisc	0.0108529	Paxs	188.53	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=R568626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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