

5,5-Dimethyl-1,3-hexadiene

Inchi:	InChI=1S/C8H14/c1-5-6-7-8(2,3)4/h5-7H,1H2,2-4H3/b7-6+
InchiKey:	YKCQGTKPNABNLF-VOTSOKGWSA-N
Formula:	C8H14
SMILES:	C=CC=CC(C)(C)C
Mol. weight [g/mol]:	110.20
CAS:	1515-79-3

Physical Properties

Property code	Value	Unit	Source
gf	187.38	kJ/mol	Joback Method
hf	25.45	kJ/mol	Joback Method
hfus	7.98	kJ/mol	Joback Method
hvap	31.39	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.775		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	380.05	K	Joback Method
tc	567.46	K	Joback Method
tf	175.50	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.55	J/molxK	380.05	Joback Method
cpg	218.53	J/molxK	411.29	Joback Method
cpg	231.69	J/molxK	442.52	Joback Method
cpg	244.08	J/molxK	473.76	Joback Method
cpg	255.73	J/molxK	504.99	Joback Method
cpg	266.69	J/molxK	536.23	Joback Method
cpg	276.99	J/molxK	567.46	Joback Method
dvisc	0.0091895	Paxs	175.50	Joback Method
dvisc	0.0029792	Paxs	209.59	Joback Method

dvisc	0.0013237	Paxs	243.68	Joback Method
dvisc	0.0007177	Paxs	277.77	Joback Method
dvisc	0.0004449	Paxs	311.87	Joback Method
dvisc	0.0003030	Paxs	345.96	Joback Method
dvisc	0.0002211	Paxs	380.05	Joback Method

Sources

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=C1515793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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