

1,4-Hexadiene, 2,5-dimethyl-

Inchi:	InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h6H,1,5H2,2-4H3
InchiKey:	JRFKHZNULLDOGQ-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	C=C(C)CC=C(C)C
Mol. weight [g/mol]:	110.20
CAS:	927-97-9

Physical Properties

Property code	Value	Unit	Source
gf	167.44	kJ/mol	Joback Method
hf	14.62	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	32.85	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	389.70 ± 2.00	K	NIST Webbook
tc	565.66	K	Joback Method
tf	145.16	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.45	J/mol×K	383.04	Joback Method
cpg	216.23	J/mol×K	413.48	Joback Method
cpg	228.39	J/mol×K	443.91	Joback Method
cpg	239.96	J/mol×K	474.35	Joback Method
cpg	250.96	J/mol×K	504.79	Joback Method
cpg	261.42	J/mol×K	535.22	Joback Method
cpg	271.37	J/mol×K	565.66	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=C927979&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
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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