

1,5-Heptadiene, 3,6-dimethyl-

Inchi:	InChI=1S/C9H16/c1-5-9(4)7-6-8(2)3/h5-6,9H,1,7H2,2-4H3
InchiKey:	JNUKYTOGXQONSJ-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	C=CC(C)CC=C(C)C
Mol. weight [g/mol]:	124.22
CAS:	34891-10-6

Physical Properties

Property code	Value	Unit	Source
gf	181.97	kJ/mol	Joback Method
hf	-1.51	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	34.61	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	407.80 ± 2.00	K	NIST Webbook
tc	587.83	K	Joback Method
tf	155.39	K	Joback Method
vc	0.495	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.59	J/mol×K	405.60	Joback Method
cpg	256.69	J/mol×K	435.97	Joback Method
cpg	270.12	J/mol×K	466.34	Joback Method
cpg	282.90	J/mol×K	496.71	Joback Method
cpg	295.05	J/mol×K	527.08	Joback Method
cpg	306.62	J/mol×K	557.46	Joback Method
cpg	317.61	J/mol×K	587.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C34891106&Units=SI

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
mccvol:	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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