

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

Other names:	5,5-dimethyl-1,3-heptadiene
Inchi:	InChI=1S/C9H16/c1-5-7-8-9(3,4)6-2/h5,7-8H,1,6H2,2-4H3/b8-7+
InchiKey:	WJRREHJZVOKKFR-BQYQJAHWSA-N
Formula:	C9H16
SMILES:	C=CC=CC(C)(C)CC
Mol. weight [g/mol]:	124.22
CAS:	24618-86-8

Physical Properties

Property code	Value	Unit	Source
gf	195.80	kJ/mol	Joback Method
hf	4.81	kJ/mol	Joback Method
hfus	10.57	kJ/mol	Joback Method
hvap	33.62	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
tb	402.93	K	Joback Method
tc	589.19	K	Joback Method
tf	186.77	K	Joback Method
vc	0.489	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.19	J/mol×K	402.93	Joback Method
cpg	259.21	J/mol×K	433.97	Joback Method
cpg	273.39	J/mol×K	465.02	Joback Method
cpg	286.75	J/mol×K	496.06	Joback Method
cpg	299.35	J/mol×K	527.10	Joback Method
cpg	311.22	J/mol×K	558.15	Joback Method
cpg	322.41	J/mol×K	589.19	Joback Method
dvisc	0.0092550	Paxs	186.77	Joback Method

dvisc	0.0029785	Paxs	222.80	Joback Method
dvisc	0.0013143	Paxs	258.82	Joback Method
dvisc	0.0007083	Paxs	294.85	Joback Method
dvisc	0.0004367	Paxs	330.88	Joback Method
dvisc	0.0002961	Paxs	366.90	Joback Method
dvisc	0.0002152	Paxs	402.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C24618868&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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