

1,3,5-Hexatriene, 3-methyl-, (E)-

Other names:	trans-3-Methyl-1,3,5-Hexatriene
Inchi:	InChI=1S/C7H10/c1-4-6-7(3)5-2/h4-6H,1-2H2,3H3/b7-6+
InchiKey:	NEVFABBVOIJXHE-VOTSOKGWSA-N
Formula:	C7H10
SMILES:	C=CC=C(C)C=C
Mol. weight [g/mol]:	94.15
CAS:	24587-26-6

Physical Properties

Property code	Value	Unit	Source
gf	255.41	kJ/mol	Joback Method
hf	170.48	kJ/mol	Joback Method
hfus	10.22	kJ/mol	Joback Method
hvap	29.87	kJ/mol	Joback Method
ie	8.28	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.305		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	356.96	K	Joback Method
tc	540.47	K	Joback Method
tf	146.09	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.04	J/mol×K	356.96	Joback Method
cpg	163.74	J/mol×K	387.54	Joback Method
cpg	173.85	J/mol×K	418.13	Joback Method
cpg	183.43	J/mol×K	448.71	Joback Method
cpg	192.47	J/mol×K	479.30	Joback Method
cpg	201.03	J/mol×K	509.88	Joback Method
cpg	209.12	J/mol×K	540.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24587266&Units=SI
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

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
ie:	Ionization energy
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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