2,2-Dimethyl-1,3,5-hexatriene

Inchi: InChI=1S/C8H12/c1-5-7-8(3,4)6-2/h6-7H,1-2H2,3-4H3
InchiKey: TVHRYPGHCFZCEZ-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=C=CC(C)(C)C=C
Mol. weight [g/mol]: 108.18
CAS: 57342-48-0

Physical Properties

Property code	Value	Unit	Source
gf	323.28	kJ/mol	Joback Method
hf	196.44	kJ/mol	Joback Method
hfus	8.63	kJ/mol	Joback Method
hvap	31.20	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.540		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	375.84	K	Joback Method
tc	569.87	K	Joback Method
tf	185.33	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.09	J/mol×K	375.84	Joback Method
cpg	208.60	J/mol×K	408.18	Joback Method
cpg	220.45	J/mol×K	440.52	Joback Method
cpg	231.67	J/mol×K	472.86	Joback Method
cpg	242.28	J/mol×K	505.20	Joback Method
cpg	252.30	J/mol×K	537.53	Joback Method
cpg	261.77	J/mol×K	569.87	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=C57342480&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