1,6-Dimethylhepta-1,3,5-triene

Other names: (E)-2,6-Dimethyl-1,3,5-heptatriene
Inchi: InChI=1S/C9H14/c1-8(2)6-5-7-9(3)4/h5-7H,1H2,2-4H3/b6-5+
InchiKey: UTPOSGXXIJEVFD-AATRIKPKSA-N
Formula: C9H14
SMILES: C=C(C)C=CC=C(C)C
Mol. weight [g/mol]: 122.21

Physical Properties

Property code	Value	Unit	Source
gf	256.08	kJ/mol	Joback Method
hf	111.20	kJ/mol	Joback Method
hfus	15.57	kJ/mol	Joback Method
hvap	35.03	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.085		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook
tb	410.08	K	Joback Method
tc	601.06	K	Joback Method
tf	151.35	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.75	J/mol×K	410.08	Joback Method
cpg	241.46	J/mol×K	441.91	Joback Method
cpg	254.41	J/mol×K	473.74	Joback Method
cpg	266.62	J/mol×K	505.57	Joback Method
cpg	278.15	J/mol×K	537.40	Joback Method
cpg	289.03	J/mol×K	569.23	Joback Method
cpg	299.30	J/mol×K	601.06	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=U196610&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume