2,3,4-Hexatriene, 2,5-dimethyl-

Inchi: InChI=1S/C8H12/c1-7(2)5-6-8(3)4/h1-4H3
InchiKey: SOESISOWJSWAJZ-UHFFFAOYSA-N
Formula: C8H12
SMILES: CC(C)=C=C=C(C)C
Mol. weight [g/mol]: 108.18
CAS: 2431-31-4

Physical Properties

Property code	Value	Unit	Source
gf	336.16	kJ/mol	Joback Method
hf	214.75	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	34.39	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	392.90	K	Joback Method
tc	596.39	K	Joback Method
tf	159.94	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.64	J/mol×K	392.90	Joback Method
cpg	210.92	J/mol×K	426.81	Joback Method
cpg	221.81	J/mol×K	460.73	Joback Method
cpg	232.29	J/mol×K	494.64	Joback Method
cpg	242.38	J/mol×K	528.56	Joback Method
cpg	252.07	J/mol×K	562.47	Joback Method
cpg	261.36	J/mol×K	596.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2431314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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