4,4-Dimethyl-1,2,5,6-heptatriene

Inchi: InChI=1S/C9H12/c1-5-7-9(3,4)8-6-2/h7-8H,1-2H2,3-4H3
InchiKey: LAUMUDIRLSPOKG-UHFFFAOYSA-N
Formula: C9H12
SMILES: C=C=CC(C)(C)C=C=C
Mol. weight [g/mol]: 120.19
CAS: 111869-19-3

Physical Properties

Property code	Value	Unit	Source
gf	459.98	kJ/mol	Joback Method
hf	340.00	kJ/mol	NIST Webbook
hfus	13.35	kJ/mol	Joback Method
hvap	33.86	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.695		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	401.99	K	Joback Method
tc	607.63	K	Joback Method
tf	203.11	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.33	J/mol×K	401.99	Joback Method
cpg	237.09	J/mol×K	436.26	Joback Method
cpg	249.21	J/mol×K	470.54	Joback Method
cpg	260.72	J/mol×K	504.81	Joback Method
cpg	271.63	J/mol×K	539.08	Joback Method
cpg	281.97	J/mol×K	573.36	Joback Method
cpg	291.74	J/mol×K	607.63	Joback Method

Sources

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=C111869193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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