1,3,6-Heptatriene, 2,5,6-trimethyl-

Other names:	2,5,6-Trimethyl-1,3,6-heptatriene
	2,5,6-Trimethyl-hepta-1,3,6-triene
	Hepta-1,3,6-triene, 2,5,6-trimethyl
Inchi:	InChI=1S/C10H16/c1-8(2)6-7-10(5)9(3)4/h6-7,10H,1,3H2,2,4-5H3/b7-6+
InchiKey:	PSZBPDGPFVFTSW-VOTSOKGWSA-N
Formula:	C10H16
SMILES:	C=C(C)C=CC(C)C(=C)C
Mol. weight [g/mol]:	136.23
CAS:	42123-66-0

Physical Properties

Property code	Value	Unit	Source
gf	269.68	kJ/mol	Joback Method
hf	93.49	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	36.24	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.331		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	425.04	K	Joback Method
tc	613.42	K	Joback Method
tf	150.94	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.95	J/mol×K	425.04	Joback Method
cpg	282.78	J/mol×K	456.44	Joback Method
cpg	296.84	J/mol×K	487.83	Joback Method
cpg	310.16	J/mol×K	519.23	Joback Method
cpg	322.78	J/mol×K	550.63	Joback Method
cpg	334.72	J/mol×K	582.02	Joback Method

cpg	346.04	J/mol×K	613.42	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42123660&Units=SI

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