1,3,6-Heptatriene, 5-methyl-

Other names: CH2=CHCH=CHCH(CH3)CH=CH2
5-Methyl-1,3,6-heptatriene
Inchi: InChI=1S/C8H12/c1-4-6-7-8(3)5-2/h4-8H,1-2H2,3H3/b7-6+
InchiKey: NDRUXLROLQGDNL-VOTSOKGWSA-N
Formula: C8H12
SMILES: C=CC=CC(C)C=C
Mol. weight [g/mol]: 108.18
CAS: 925-52-0

Physical Properties

Property code	Value	Unit	Source
gf	269.94	kJ/mol	Joback Method
hf	154.35	kJ/mol	Joback Method
hfus	10.59	kJ/mol	Joback Method
hvap	31.63	kJ/mol	Joback Method
ie	8.40 ± 0.10	eV	NIST Webbook
log10ws	-2.49		Crippen Method
logp	2.551		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
ripol	1549.00		NIST Webbook
tb	379.52	K	Joback Method
tc	563.02	K	Joback Method
tf	156.32	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.98	J/mol×K	379.52	Joback Method
cpg	243.69	J/mol×K	532.44	Joback Method
cpg	233.90	J/mol×K	501.86	Joback Method
cpg	223.57	J/mol×K	471.27	Joback Method
cpg	212.66	J/mol×K	440.69	Joback Method

cpg	201.14	J/mol×K	410.10	Joback Method
cpg	252.94	J/mol×K	563.02	Joback Method
dvisc	0.0001842	Pa×s	379.52	Joback Method
dvisc	0.0002416	Pa×s	342.32	Joback Method
dvisc	0.0003385	Pa×s	305.12	Joback Method
dvisc	0.0005210	Pa×s	267.92	Joback Method
dvisc	0.0009214	Pa×s	230.72	Joback Method
dvisc	0.0020289	Pa×s	193.52	Joback Method
dvisc	0.0065053	Pa×s	156.32	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=C925520&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
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: