1,2,5-Hexatriene

Inchi: InChI=1S/C6H8/c1-3-5-6-4-2/h3,6H,1-2,5H2
InchiKey: KHQKGRVDIZQGHT-UHFFFAOYSA-N
Formula: C6H8
SMILES: C=C=CCC=C
Mol. weight [g/mol]: 80.13
CAS: 116377-11-8

Physical Properties

Property code	Value	Unit	Source
gf	303.60	kJ/mol	Joback Method
hf	246.47	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	28.05	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.904		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	333.31	K	Joback Method
tc	515.51	K	Joback Method
tf	160.37	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.23	J/mol×K	333.31	Joback Method
cpg	135.14	J/mol×K	363.68	Joback Method
cpg	142.76	J/mol×K	394.04	Joback Method
cpg	150.10	J/mol×K	424.41	Joback Method
cpg	157.16	J/mol×K	454.77	Joback Method
cpg	163.95	J/mol×K	485.14	Joback Method
cpg	170.47	J/mol×K	515.51	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=C116377118&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