5-Methyl-1-phenylhexa-1,3,4-triene

Inchi: InChI=1S/C13H14/c1-12(2)8-6-7-11-13-9-4-3-5-10-13/h3-7,9-11H,1-2H3/b11-7+
InchiKey: ODCHZOADCIUBBE-YRNVUSSQSA-N
Formula: C13H14
SMILES: CC(C)=C=CC=Cc1ccccc1
Mol. weight [g/mol]: 170.25
CAS: 103240-79-5

Physical Properties

Property code	Value	Unit	Source
gf	451.16	kJ/mol	Joback Method
hf	312.31	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	47.24	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.821		Crippen Method
mcvol	157.370	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	534.99	K	Joback Method
tc	767.46	K	Joback Method
tf	245.08	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.18	J/mol×K	534.99	Joback Method
cpg	357.78	J/mol×K	573.74	Joback Method
cpg	373.25	J/mol×K	612.48	Joback Method
cpg	387.64	J/mol×K	651.23	Joback Method
cpg	401.04	J/mol×K	689.97	Joback Method
cpg	413.52	J/mol×K	728.72	Joback Method
cpg	425.15	J/mol×K	767.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103240795&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
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