Spiro[2,4]hepta-4,6-diene

Other names: Spiro[2.4]hepta-4,6-diene
Inchi: InChI=1S/C7H8/c1-2-4-7(3-1)5-6-7/h1-4H,5-6H2
InchiKey: KPDOKSJMJMDRQA-UHFFFAOYSA-N
Formula: C7H8
SMILES: C1=CC2(C=C1)CC2
Mol. weight [g/mol]: 92.14
CAS: 765-46-8

Physical Properties

Property code	Value	Unit	Source
gf	179.60	kJ/mol	Joback Method
hf	238.00	kJ/mol	NIST Webbook
hfus	3.13	kJ/mol	Joback Method
hvap	30.92	kJ/mol	Joback Method
ie	8.14	eV	NIST Webbook
log10ws	-2.01		Crippen Method
logp	1.893		Crippen Method
mcvol	79.170	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
tb	380.54	K	Joback Method
tc	598.56	K	Joback Method
tf	230.67	K	Joback Method
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.28	J/mol×K	380.54	Joback Method
cpg	150.62	J/mol×K	416.88	Joback Method
cpg	163.39	J/mol×K	453.21	Joback Method
cpg	174.75	J/mol×K	489.55	Joback Method
cpg	184.88	J/mol×K	525.89	Joback Method
cpg	193.94	J/mol×K	562.23	Joback Method
cpg	202.09	J/mol×K	598.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.20	K	13.30	NIST Webbook

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=C765468&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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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