6,6-Diphenylfulvene

Other names:	Benzene, (2,4-cyclopentadien-1-ylidenephenylmethyl)-
	Methane, 2,4-cyclopentadien-1-ylidenediphenyl-
	Diphenylfulvene
	Diphenylmethylidene cyclopentadiene
	5-(Diphenylmethylene)-1,3-cyclopentadiene
	Fulvene, 6,6-diphenyl
	6,6'-diphenylfulvene
Inchi:	InChI=1S/C18H14/c1-3-9-15(10-4-1)18(17-13-7-8-14-17)16-11-5-2-6-12-16/h1-14H
InchiKey:	BULLHRADHZGONG-UHFFFAOYSA-N
Formula:	C18H14
SMILES:	C1=CC(=C(c2ccccc2)c2ccccc2)C=C1
Mol. weight [g/mol]:	230.30
CAS:	2175-90-8

Physical Properties

Property code	Value	Unit	Source
chs	-9381.00 ± 13.00	kJ/mol	NIST Webbook
gf	466.59	kJ/mol	Joback Method
hf	320.83	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hsub	100.00	kJ/mol	NIST Webbook
hvap	62.23	kJ/mol	Joback Method
ie	7.96	eV	NIST Webbook
log10ws	-5.29		Crippen Method
logp	4.614		Crippen Method
mcvol	193.200	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
tb	689.39	K	Joback Method
tc	959.12	K	Joback Method
tf	358.52	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.71	J/mol×K	689.39	Joback Method
cpg	512.66	J/mol×K	734.34	Joback Method
cpg	528.94	J/mol×K	779.30	Joback Method
cpg	543.72	J/mol×K	824.25	Joback Method
cpg	557.21	J/mol×K	869.21	Joback Method
cpg	569.57	J/mol×K	914.16	Joback Method
cpg	580.98	J/mol×K	959.12	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=C2175908&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
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
hsub: Enthalpy of sublimation 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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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