1,1'-Diphenyl-1,1'-bicyclopentyl

Inchi: InChI=1S/C22H26/c1-3-11-19(12-4-1)21(15-7-8-16-21)22(17-9-10-18-22)20-13-5-2-6-14-
InchiKey: MJIRQUDRSKNXSM-UHFFFAOYSA-N
Formula: C22H26
SMILES: c1ccc(C2(C3(c4ccccc4)CCCC3)CCCC2)cc1
Mol. weight [g/mol]: 290.44
CAS: 59358-70-2

Physical Properties

Property code	Value	Unit	Source
chs	-12343.00 ± 1.00	kJ/mol	NIST Webbook
gf	421.30	kJ/mol	Joback Method
hf	111.00 ± 2.20	kJ/mol	NIST Webbook
hfs	-30.00 ± 1.00	kJ/mol	NIST Webbook
hfus	16.09	kJ/mol	Joback Method
hsub	141.00	kJ/mol	NIST Webbook
hsub	141.00	kJ/mol	NIST Webbook
hvap	67.33	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.010		Crippen Method
mcvol	251.600	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	787.16	K	Joback Method
tc	1068.88	K	Joback Method
tf	414.00 ± 1.00	K	NIST Webbook
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.90	J/mol×K	787.16	Joback Method
cpg	804.48	J/mol×K	834.11	Joback Method
cpg	830.56	J/mol×K	881.07	Joback Method
cpg	856.76	J/mol×K	928.02	Joback Method
cpg	883.68	J/mol×K	974.97	Joback Method

cpg	911.92	J/mol×K	1021.93	Joback Method
cpg	942.11	J/mol×K	1068.88	Joback Method
cps	375.50	J/mol×K	298.00	NIST Webbook
hfust	31.38	kJ/mol	414.00	NIST Webbook
hsubt	141.40	kJ/mol	141.40	NIST Webbook

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=C59358702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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