1,1'-Diphenyl-1,1'-bicyclohexyl

Inchi: InChI=1S/C24H30/c1-5-13-21(14-6-1)23(17-9-3-10-18-23)24(19-11-4-12-20-24)22-15-7-2
InchiKey: SZGBUFROANKUNE-UHFFFAOYSA-N
Formula: C24H30
SMILES: c1ccc(C2(C3(c4ccccc4)CCCCC3)CCCCC2)cc1
Mol. weight [g/mol]: 318.50
CAS: 59358-71-3

Physical Properties

Property code	Value	Unit	Source
chs	-13624.80 ± 1.60	kJ/mol	NIST Webbook
gf	413.94	kJ/mol	Joback Method
hf	44.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-106.90 ± 1.60	kJ/mol	NIST Webbook
hfus	17.07	kJ/mol	Joback Method
hsub	150.90	kJ/mol	NIST Webbook
hsub	150.00	kJ/mol	NIST Webbook
hvap	72.13	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.791		Crippen Method
mcvol	279.780	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
tb	841.46	K	Joback Method
tc	1125.89	K	Joback Method
tf	455.00 ± 1.00	K	NIST Webbook
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.95	J/mol×K	1078.48	Joback Method
cpg	907.46	J/mol×K	841.46	Joback Method
cpg	936.72	J/mol×K	888.86	Joback Method
cpg	965.70	J/mol×K	936.27	Joback Method
cpg	995.00	J/mol×K	983.67	Joback Method

cpg	1025.21	J/mol×K	1031.08	Joback Method
cpg	1090.80	J/mol×K	1125.89	Joback Method
cps	403.80	J/mol×K	298.00	NIST Webbook
hfust	29.71	kJ/mol	455.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59358713&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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