2,6-Diphenyl-thiacyclohexanone-4

Inchi: InChI=1S/C17H16OS/c18-15-11-16(13-7-3-1-4-8-13)19-17(12-15)14-9-5-2-6-10-14/h1-10
InchiKey: PPJHHCQGZVIWAR-UHFFFAOYSA-N
Formula: C17H16OS
SMILES: O=C1CC(c2ccccc2)SC(c2ccccc2)C1
Mol. weight [g/mol]: 268.37
CAS: 37014-01-0

Physical Properties

Property code	Value	Unit	Source
chs	-9491.80 ± 9.70	kJ/mol	NIST Webbook
chs	-9518.60 ± 6.70	kJ/mol	NIST Webbook
gf	251.09	kJ/mol	Joback Method
hf	84.10 ± 7.40	kJ/mol	NIST Webbook
hfus	23.94	kJ/mol	Joback Method
hsub	144.00	kJ/mol	NIST Webbook
hsub	144.00 ± 3.00	kJ/mol	NIST Webbook
hvap	68.17	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.565		Crippen Method
mcvol	209.930	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
tb	772.25	K	Joback Method
tc	1060.09	K	Joback Method
tf	489.00	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.95	J/mol×K	772.25	Joback Method
cpg	620.79	J/mol×K	820.22	Joback Method
cpg	638.46	J/mol×K	868.20	Joback Method
cpg	654.05	J/mol×K	916.17	Joback Method
cpg	667.63	J/mol×K	964.14	Joback Method

cpg	679.29	J/mol×K	1012.11	Joback Method
cpg	689.09	J/mol×K	1060.09	Joback Method
hsubt	136.00	kJ/mol	375.00	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=C37014010&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
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
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