Cyclohexanone, 6-[(butylthio)methylene]-2,2-diphenyl-

Inchi: InChI=1S/C23H26OS/c1-2-3-17-25-18-19-11-10-16-23(22(19)24,20-12-6-4-7-13-20)21-1

InchiKey: DJPZTHCPTYZSHM-HNENSFHCSA-N

Formula: C23H26OS

SMILES: CCCCSC=C1CCCC(c2ccccc2)(c2ccccc2)C1=O

Mol. weight [g/mol]: 350.52

CAS: 50592-51-3

Physical Properties

Property code	Value	Unit	Source
gf	342.55	kJ/mol	Joback Method
hf	4.77	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.143		Crippen Method
mcvol	290.170	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
tb	942.03	K	Joback Method
tc	1212.32	K	Joback Method
tf	546.07	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.63	J/mol×K	942.03	Joback Method
cpg	947.01	J/mol×K	987.08	Joback Method
cpg	967.74	J/mol×K	1032.13	Joback Method
cpg	988.07	J/mol×K	1077.18	Joback Method
cpg	1008.27	J/mol×K	1122.22	Joback Method
cpg	1028.60	J/mol×K	1167.27	Joback Method
cpg	1049.33	J/mol×K	1212.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50592513&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

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
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