2,6-Diphenyltetrahydrothiopyran-4-one s,s-dioxide

Inchi: InChI=1S/C17H16O3S/c18-15-11-16(13-7-3-1-4-8-13)21(19,20)17(12-15)14-9-5-2-6-10-1

InchiKey: UEPWZKMHEHTBRW-UHFFFAOYSA-N

Formula: C17H16O3S

SMILES: O=C1CC(c2ccccc2)S(=O)(=O)C(c2ccccc2)C1

Mol. weight [g/mol]: 300.37

CAS: 103225-43-0

Physical Properties

Property code	Value	Unit	Source
chs	-9157.00 ± 12.00	kJ/mol	NIST Webbook
gf	-250.57	kJ/mol	Joback Method
hf	-474.83	kJ/mol	Joback Method
hfus	31.19	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.247		Crippen Method
mcvol	221.670	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
tb	751.25	K	Joback Method
tc	1008.85	K	Joback Method
tf	493.16	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.89	J/mol×K	751.25	Joback Method
cpg	653.25	J/mol×K	794.18	Joback Method
cpg	670.62	J/mol×K	837.12	Joback Method
cpg	686.05	J/mol×K	880.05	Joback Method
cpg	699.56	J/mol×K	922.98	Joback Method
cpg	711.21	J/mol×K	965.92	Joback Method
cpg	721.04	J/mol×K	1008.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103225430&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
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