

(Z) 1,3-Diphenyl-3-thioxo-1-propen-1-ol

Inchi:	InChI=1S/C15H12OS/c16-14(12-7-3-1-4-8-12)11-15(17)13-9-5-2-6-10-13/h1-11,16H/b14
InchiKey:	UAHPEAKMUKHDAA-KAMYIIQDSA-N
Formula:	C15H12OS
SMILES:	OC(=CC(=S)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	240.32
CAS:	61520-36-3

Physical Properties

Property code	Value	Unit	Source
gf	352.15	kJ/mol	Joback Method
hf	221.83	kJ/mol	Joback Method
hfus	30.27	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.004		Crippen Method
mcvol	188.310	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	762.22	K	Joback Method
tc	1010.22	K	Joback Method
tf	387.70	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.94	J/molxK	762.22	Joback Method
cpg	491.79	J/molxK	803.55	Joback Method
cpg	502.76	J/molxK	844.89	Joback Method
cpg	513.01	J/molxK	886.22	Joback Method
cpg	522.71	J/molxK	927.56	Joback Method
cpg	532.01	J/molxK	968.89	Joback Method
cpg	541.09	J/molxK	1010.22	Joback Method

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=C61520363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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