(Z)
1-(4-Methoxyphenyl)-3-phenyl-3-thioxo-1-propen-

Inchi: InChI=1S/C16H14O2S/c1-18-14-9-7-12(8-10-14)15(17)11-16(19)13-5-3-2-4-6-13/h2-11,1

InchiKey: IJXXYIYPKAEPGP-PTNGSMBKSA-N

Formula: C16H14O2S

SMILES: COc1ccc(C(O)=CC(=S)c2ccccc2)cc1

Mol. weight [g/mol]: 270.35

CAS: 76526-09-5

Physical Properties

Property code	Value	Unit	Source
gf	245.94	kJ/mol	Joback Method
hf	57.50	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	82.28	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.012		Crippen Method
mcvol	208.270	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
tb	812.50	K	Joback Method
tc	1053.00	K	Joback Method
tf	433.72	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.89	J/mol×K	812.50	Joback Method
cpg	567.86	J/mol×K	852.58	Joback Method
cpg	579.03	J/mol×K	892.67	Joback Method
cpg	589.52	J/mol×K	932.75	Joback Method
cpg	599.44	J/mol×K	972.83	Joback Method
cpg	608.93	J/mol×K	1012.91	Joback Method
cpg	618.09	J/mol×K	1053.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76526095&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