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

Inchi: InChI=1S/C15H11BrOS/c16-13-8-6-11(7-9-13)14(17)10-15(18)12-4-2-1-3-5-12/h1-10,17H

InchiKey: KREPOKDTPLAMIN-UVTDQMKNSA-N

Formula: C15H11BrOS

SMILES: OC(=CC(=S)c1ccccc1)c1ccc(Br)cc1

Mol. weight [g/mol]: 319.22

CAS: 76526-07-3

Physical Properties

Property code	Value	Unit	Source
gf	356.84	kJ/mol	Joback Method
hf	236.69	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.766		Crippen Method
mcvol	205.810	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	833.36	K	Joback Method
tc	1091.05	K	Joback Method
tf	460.02	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.81	J/mol×K	833.36	Joback Method
cpg	517.28	J/mol×K	876.31	Joback Method
cpg	527.17	J/mol×K	919.26	Joback Method
cpg	536.68	J/mol×K	962.21	Joback Method
cpg	546.00	J/mol×K	1005.15	Joback Method
cpg	555.32	J/mol×K	1048.10	Joback Method
cpg	564.81	J/mol×K	1091.05	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=C76526073&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