Ethanone, 1-[4-(phenylthio)phenyl]-

Other names:	4-Phenylthioacetophenone
	1-[4-(phenylthio)phenyl]ethan-1-one
Inchi:	InChI=1S/C14H12OS/c1-11(15)12-7-9-14(10-8-12)16-13-5-3-2-4-6-13/h2-10H,1H3
InchiKey:	XUDYHODVSUXRPW-UHFFFAOYSA-N
Formula:	C14H12OS
SMILES:	CC(=O)c1ccc(Sc2ccccc2)cc1
Mol. weight [g/mol]:	228.31
CAS:	10169-55-8

Physical Properties

Property code	Value	Unit	Source
gf	186.39	kJ/mol	Joback Method
hf	58.59	kJ/mol	Joback Method
hfus	25.44	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.040		Crippen Method
mcvol	178.520	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	700.71	K	Joback Method
tc	965.53	K	Joback Method
tf	397.23	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.20	J/mol×K	700.71	Joback Method
cpg	456.00	J/mol×K	744.85	Joback Method
cpg	469.43	J/mol×K	788.98	Joback Method
cpg	481.57	J/mol×K	833.12	Joback Method
cpg	492.50	J/mol×K	877.26	Joback Method
cpg	502.29	J/mol×K	921.40	Joback Method
cpg	511.01	J/mol×K	965.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10169558&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

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