

4-Phenylthioacetophenone

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]:	228.32

Physical Properties

Property code	Value	Unit	Source
af	0.4651		Cheméo Relay (1.0)
gf	186.39	kJ/mol	Joback Method
hf	25.37	kJ/mol	Cheméo Relay (1.0)
hfus	25.44	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-4.66		Cheméo Relay (1.0)
logp	4.040		Crippen Method
mcvol	178.520	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	643.40	K	Cheméo Relay (1.0)
tc	869.92	K	Cheméo Relay (1.0)
tf	358.95	K	Cheméo Relay (1.0)
vc	0.631	m3/kmol	Cheméo Relay (1.0)

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10169558&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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