1-Phenylthio-3-acetoxy-2-butanone

Inchi: InChI=1S/C12H14O3S/c1-9(15-10(2)13)12(14)8-16-11-6-4-3-5-7-11/h3-7,9H,8H2,1-2H3
InchiKey: ATXBBUJVWLXBJK-UHFFFAOYSA-N
Formula: C12H14O3S
SMILES: CC(=O)OC(C)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 238.30
CAS: 67175-41-1

Physical Properties

Property code	Value	Unit	Source
gf	-169.59	kJ/mol	Joback Method
hf	-375.27	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.299		Crippen Method
mcvol	181.540	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	699.14	K	Joback Method
tc	932.53	K	Joback Method
tf	392.91	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.72	J/mol×K	699.14	Joback Method
cpg	478.35	J/mol×K	738.04	Joback Method
cpg	490.93	J/mol×K	776.94	Joback Method
cpg	502.47	J/mol×K	815.83	Joback Method
cpg	512.98	J/mol×K	854.73	Joback Method
cpg	522.50	J/mol×K	893.63	Joback Method
cpg	531.03	J/mol×K	932.53	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=C67175411&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