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]: 238.31

Physical Properties

Property code	Value	Unit	Source
hf	-459.31	kJ/mol	Cheméo Relay (1.0)
hfus	25.87	kJ/mol	Joback Method
logp	2.299		Crippen Method
mcvol	181.540	ml/mol	McGowan Method
tf	352.45	K	Cheméo Relay (1.0)

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
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=C67175411&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point