2-Propanone, 1-[(4-methylphenyl)sulfonyl]-

Other names:	2-Propanone, 1-(p-tolylsulfonyl)-
	(p-Tolylsulfonyl)acetone
	1-(p-Tolylsulfonyl)-2-propanone
	p-Toluenesulfonylacetone
	4-Toluenesulfonylacetone
	(p-tolylsulphonyl)acetone
Inchi:	InChI=1S/C10H12O3S/c1-8-3-5-10(6-4-8)14(12,13)7-9(2)11/h3-6H,7H2,1-2H3
InchiKey:	NDQXJNHOGLQSMB-UHFFFAOYSA-N
Formula:	C10H12O3S
SMILES:	CC(=O)CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	212.26
CAS:	5366-49-4

Physical Properties

Property code	Value	Unit	Source
gf	-461.36	kJ/mol	Joback Method
hf	-590.60	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.358		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	561.51	K	Joback Method
tc	769.73	K	Joback Method
tf	329.89	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.07	J/mol×K	561.51	Joback Method
cpg	369.75	J/mol×K	596.21	Joback Method
cpg	382.63	J/mol×K	630.92	Joback Method

cpg	394.70	J/mol×K	665.62	Joback Method
cpg	405.99	J/mol×K	700.33	Joback Method
cpg	416.49	J/mol×K	735.03	Joback Method
cpg	426.23	J/mol×K	769.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5366494&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