Phenyl sulfonyl acetone

Other names:	1-Methyl-2-phenylsulfonylethanone
	2-Propanone, 1-(phenylsulfonyl)-
	2-Propanone, (phenylsulfonyl)-
	Phenylsulfonylacetylmethane
	1-(Phenylsulfonyl)-2-propanone
	Phenylsulphonylacetone
Inchi:	InChI=1S/C9H10O3S/c1-8(10)7-13(11,12)9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	YBLGSNMIIPIRFC-UHFFFAOYSA-N
Formula:	C9H10O3S
SMILES:	CC(=O)CS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	198.24
CAS:	5000-44-2

Physical Properties

Property code	Value	Unit	Source
gf	-460.15	kJ/mol	Joback Method
hf	-558.49	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.049		Crippen Method
mcvol	143.570	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	533.65	K	Joback Method
tc	744.14	K	Joback Method
tf	306.10	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.53	J/mol×K	533.65	Joback Method
cpg	323.70	J/mol×K	568.73	Joback Method
cpg	336.06	J/mol×K	603.81	Joback Method

cpg	347.62	J/mol×K	638.89	Joback Method
cpg	358.40	J/mol×K	673.97	Joback Method
cpg	368.41	J/mol×K	709.06	Joback Method
cpg	377.66	J/mol×K	744.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5000442&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

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