2-(P-TOLYLSULFONYL)ACETOPHENONE

Other names:	(p-Tolylsulfonyl)benzoylmethane
	2-(p-Toluenesulfonyl)acetophenone
	2-[(4-methylphenyl)sulphonyl]-1-phenylethan-1-one
	4-Methylphenyl phenacyl sulfone
	Acetophenone, 2-(p-tolylsulfonyl)-
	Ethanone, 2-[(4-methylphenyl)sulfonyl]-1-phenyl-
	NSC 140338
	Phenacyl p-tolyl sulfone
	p-Tolyl phenacyl sulfone
	«alpha»-(4-Toluenesulfonyl)acetophenone
	«alpha»-(4-Toluenesulphonyl)acetophenone
	«alpha»-(p-Toluenesulfonyl)acetophenone
	«alpha»-(p-Tolylsulfonyl)acetophenone
Inchi:	InChI=1S/C15H14O3S/c1-12-7-9-14(10-8-12)19(17,18)11-15(16)13-5-3-2-4-6-13/h2-10H
InchiKey:	RFQXSRPFYWMUDV-UHFFFAOYSA-N
Formula:	C15H14O3S
SMILES:	Cc1ccc(S(=O)(=O)CC(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	274.34

Physical Properties

Property code	Value	Unit	Source
hf	-301.96	kJ/mol	Cheméo Relay (1.0)
hfus	35.28	kJ/mol	Joback Method
hvap	110.98	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-3.73		Cheméo Relay (1.0)
logp	2.652		Crippen Method
mcvol	204.350	ml/mol	McGowan Method
tb	665.76	K	Cheméo Relay (1.0)
tf	400.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	526.34	J/mol×K	702.59	Joback Method
cpg	541.44	J/mol×K	741.18	Joback Method
cpg	555.24	J/mol×K	779.77	Joback Method
cpg	567.80	J/mol×K	818.36	Joback Method
cpg	579.14	J/mol×K	856.95	Joback Method
cpg	589.32	J/mol×K	895.54	Joback Method
cpg	598.37	J/mol×K	934.12	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=C31378037&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point