

2-(p-Tolylsulfonyl)acetophenone

Other names:

«alpha»-(p-Tolylsulfonyl)acetophenone
«alpha»-(p-Toluenesulfonyl)acetophenone
«alpha»-(4-Toluenesulfonyl)acetophenone
Ethanone, 2-[(4-methylphenyl)sulfonyl]-1-phenyl-
Acetophenone, 2-(p-tolylsulfonyl)-
(p-Tolylsulfonyl)benzoylmethane
2-(p-Toluenesulfonyl)acetophenone
4-Methylphenyl phenacyl sulfone
p-Tolyl phenacyl sulfone
Phenacyl p-tolyl sulfone
«alpha»-(4-Toluenesulphonyl)acetophenone
NSC 140338
2-[(4-methylphenyl)sulphonyl]-1-phenylethan-1-one

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:

RFQXSRPFYWUDV-UHFFFAOYSA-N

Formula:

C17H18OS

SMILES:

Cc1ccc(S(=O)(=O)CC(=O)c2ccccc2)cc1

Mol. weight [g/mol]:

270.39

CAS:

31378-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-306.85	kJ/mol	Joback Method
hf	-457.27	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.652		Crippen Method
mcvol	204.350	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	702.59	K	Joback Method
tc	934.12	K	Joback Method
tf	412.66	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31378037&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

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