

Acetic acid, [(4-methylphenyl)sulfonyl]-, ethyl ester

Other names:	Acetic acid, (p-tolylsulfonyl)-, ethyl ester Ethyl 2-(para-tolylsulfonyl)-acetate Ethyl «alpha»-(p-toluenesulfonyl)acetate Ethyl «alpha»-(p-tolylsulfonyl)acetate ethyl (4-tolylsulphonyl)acetate
Inchi:	InChI=1S/C11H14O4S/c1-3-15-11(12)8-16(13,14)10-6-4-9(2)5-7-10/h4-7H,3,8H2,1-2H3
InchiKey:	VDXYJUBMHZEPOQ-UHFFFAOYSA-N
Formula:	C11H14O4S
SMILES:	CCOC(=O)CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	242.29
CAS:	2850-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-557.94	kJ/mol	Joback Method
hf	-743.46	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.332		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
tb	606.81	K	Joback Method
tc	809.82	K	Joback Method
tf	363.39	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.91	J/molxK	606.81	Joback Method
cpg	443.01	J/molxK	640.65	Joback Method
cpg	456.28	J/molxK	674.48	Joback Method
cpg	468.74	J/molxK	708.32	Joback Method

cpg	480.38	J/mol×K	742.15	Joback Method
cpg	491.20	J/mol×K	775.99	Joback Method
cpg	501.20	J/mol×K	809.82	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2850193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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