Benzenesulfonic acid, 4-methyl-, ethyl ester

Other names:	p-Toluenesulfonic acid, ethyl ester
	Ethyl p-methylbenzenesulfonate
	Ethyl p-toluenesulfonate
	Ethyl p-tosylate
	Ethyl tosylate
	Ethyl para-toluenesulfonate
	Ethyl 4-toluenesulfonate
	Ethyl toluene-4-sulfonate
	p-Toluolsulfonsaeure aethyl ester
	Ethyl p-TS
	Ethylester kyseliny p-toluensulfonove
	Ethyl ester of p-Toluenesulfonic acid
	4-Methylbenzenesulfonic acid ethyl ester
	Mittel AEP
	NSC 8887
	Toluene-4-sulfonic acid ethyl ester
	ethyl toluene-4-sulphonate
Inchi:	InChI=1S/C9H12O3S/c1-3-12-13(10,11)9-6-4-8(2)5-7-9/h4-7H,3H2,1-2H3
InchiKey:	VRZVPALEJCLXPR-UHFFFAOYSA-N
Formula:	C9H12O3S
SMILES:	CCOS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	200.25
CAS:	80-40-0

Physical Properties

Property code	Value	Unit	Source
gf	-445.86	kJ/mol	Joback Method
hf	-589.60	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.720		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	507.18	K	Joback Method
tc	707.85	K	Joback Method
tf	304.00 ± 4.00	K	NIST Webbook

tf	307.00 ± 2.00	K	NIST Webbook
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.24	J/mol×K	507.18	Joback Method
cpg	329.87	J/mol×K	540.63	Joback Method
cpg	342.86	J/mol×K	574.07	Joback Method
cpg	355.20	J/mol×K	607.52	Joback Method
cpg	366.89	J/mol×K	640.96	Joback Method
cpg	377.91	J/mol×K	674.41	Joback Method
cpg	388.27	J/mol×K	707.85	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80400&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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