

Benzenesulfonamide, N-ethyl-4-methyl-

Other names:	p-Toluenesulfonamide, N-ethyl- p-Tolueneethylsulfonamide p-Toluenesulfonyl-N-ethylamide N-Ethyl-p-methylbenzenesulfonamide N-Ethyl-p-toluenesulfonamide N-Ethyl-p-tolylsulfonamide N-Tosylethylamine Santicizer 3 N-Ethyl-4-methyl-benzenesulfonamide Ethyl toluenesulfonamide Unipex 108 Uniplex 108 4-Toluenesulfonamide, N-ethyl- N-Ethyl-4-toluenesulfonamide NSC 68803 N-ethyltoluene-4-sulphonamide
Inchi:	InChI=1S/C9H13NO2S/c1-3-10-13(11,12)9-6-4-8(2)5-7-9/h4-7,10H,3H2,1-2H3
InchiKey:	OHPZPBNDQVQJMH-UHFFFAOYSA-N
Formula:	C9H13NO2S
SMILES:	CCNS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	199.27
CAS:	80-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-251.47	kJ/mol	Joback Method
hf	-403.91	kJ/mol	Joback Method
hfus	29.20	kJ/mol	Joback Method
hvap	63.64	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.293		Crippen Method
mcvol	151.980	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	289.90		NIST Webbook
tb	534.93	K	Joback Method
tc	738.46	K	Joback Method
tf	321.35	K	Joback Method

vc	0.593	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.78	J/mol×K	534.93	Joback Method
cpg	353.84	J/mol×K	568.85	Joback Method
cpg	367.12	J/mol×K	602.77	Joback Method
cpg	379.63	J/mol×K	636.69	Joback Method
cpg	391.39	J/mol×K	670.61	Joback Method
cpg	402.39	J/mol×K	704.53	Joback Method
cpg	412.66	J/mol×K	738.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80397&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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