

Benzenesulfonamide, n,n,4-trimethyl-

Other names:	p-Toluenesulfonamide, N,N-dimethyl- N,N-Dimethyl-p-toluenesulfonamide N,N,4-Trimethyl-benzenesulfonamide 4,N,N-Trimethylbenzenesulfonamide N-[(4-Methylphenyl)sulfonyl]dimethylamine N,N-dimethyl-p-toluenesulphonamide
Inchi:	InChI=1S/C9H13NO2S/c1-8-4-6-9(7-5-8)13(11,12)10(2)3/h4-7H,1-3H3
InchiKey:	WZKOKGOAHBIPCI-UHFFFAOYSA-N
Formula:	C9H13NO2S
SMILES:	Cc1ccc(S(=O)(=O)N(C)C)cc1
Mol. weight [g/mol]:	199.28

Physical Properties

Property code	Value	Unit	Source
af	0.4946		Cheméo Relay (1.0)
gf	-230.08	kJ/mol	Joback Method
hf	-238.51	kJ/mol	Cheméo Relay (1.0)
hfus	27.12	kJ/mol	Joback Method
hvap	77.77	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-2.59		Cheméo Relay (1.0)
logp	1.245		Crippen Method
mcvol	151.980	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1671.00		NIST Webbook
tb	589.18	K	Cheméo Relay (1.0)
tc	783.86	K	Cheméo Relay (1.0)
tf	402.27	K	Cheméo Relay (1.0)
vc	0.560	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	324.95	J/mol×K	497.20	Joback Method
cpg	339.72	J/mol×K	530.47	Joback Method
cpg	353.68	J/mol×K	563.75	Joback Method
cpg	366.84	J/mol×K	597.02	Joback Method
cpg	379.24	J/mol×K	630.29	Joback Method
cpg	390.87	J/mol×K	663.57	Joback Method
cpg	401.76	J/mol×K	696.84	Joback Method

Sources

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=C599699&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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