

Benzenesulfonamide, n,4-dimethyl-

Other names:	p-Toluenesulfonamide, N-methyl- (p-Tolylsulfonyl)methylamine p-Toluene-N-methylsulfonamide N-Methyl-p-toluenesulfonamide N,4-Dimethylbenzenesulfonamide N-Methyl-para-toluenesulfonamide N-Methyl-p-toluolsulfonamide N-methyltoluene-4-sulphonamide
Inchi:	InChI=1S/C8H11NO2S/c1-7-3-5-8(6-4-7)12(10,11)9-2/h3-6,9H,1-2H3
InchiKey:	GWLOGZRVYXAHRE-UHFFFAOYSA-N
Formula:	C8H11NO2S
SMILES:	CNS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	185.25

Physical Properties

Property code	Value	Unit	Source
af	0.5368		Cheméo Relay (1.0)
gf	-259.89	kJ/mol	Joback Method
hf	-245.41	kJ/mol	Cheméo Relay (1.0)
hfus	26.61	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-1.70		Cheméo Relay (1.0)
logp	0.903		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	587.77	K	Cheméo Relay (1.0)
tc	800.50	K	Cheméo Relay (1.0)
tf	377.18	K	Cheméo Relay (1.0)
vc	0.492	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.78	J/mol×K	512.05	Joback Method
cpg	307.95	J/mol×K	546.48	Joback Method
cpg	320.40	J/mol×K	580.91	Joback Method
cpg	332.12	J/mol×K	615.34	Joback Method
cpg	343.14	J/mol×K	649.77	Joback Method
cpg	353.45	J/mol×K	684.20	Joback Method
cpg	363.06	J/mol×K	718.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C640619&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

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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