

Toluenesulfonamide, alpha-

Other names:	«alpha»-Toluenesulfonamide Benzylsulfonamide Methanesulfonamide, 1-phenyl- Phenylmethanesulfonamide Toluene-«omega»-sulfonamide Toluenesulfonamide, alpha- toluene-«alpha»-sulphonamide
Inchi:	InChI=1S/C7H9NO2S/c8-11(9,10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,8,9,10)
InchiKey:	ABOYDMHGKWRPFD-UHFFFAOYSA-N
Formula:	C7H9NO2S
SMILES:	NS(=O)(=O)Cc1ccccc1
Mol. weight [g/mol]:	171.22

Physical Properties

Property code	Value	Unit	Source
af	0.5768		Cheméo Relay (1.0)
hf	-250.51	kJ/mol	Cheméo Relay (1.0)
hfus	24.50	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-1.82		Cheméo Relay (1.0)
logp	0.475		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	5511.44	kPa	Joback Method
tb	565.94	K	Cheméo Relay (1.0)
tc	824.37	K	Cheméo Relay (1.0)
tf	411.24	K	Cheméo Relay (1.0)
vc	0.435	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.52	J/mol×K	506.55	Joback Method
cpg	273.85	J/mol×K	542.94	Joback Method

cpg	285.41	J/mol×K	579.32	Joback Method
cpg	296.20	J/mol×K	615.71	Joback Method
cpg	306.25	J/mol×K	652.10	Joback Method
cpg	315.56	J/mol×K	688.48	Joback Method
cpg	324.15	J/mol×K	724.87	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4563331&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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