

# 4-Tert-butylphenyl benzene sulfonate

**InChI:** InChI=1S/C16H18O3S/c1-16(2,3)13-9-11-14(12-10-13)19-20(17,18)15-7-5-4-6-8-15/h4-12H,1-3H3

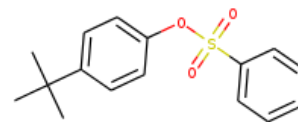
**InChI Key:** GLHUQUIUKLSAEEK-UHFFFAOYSA-N

**Formula:** C16H18O3S

**SMILES:** CC(C)(C)c1ccc(OS(=O)(=O)c2ccccc2)cc1

**Molecular Weight:** 290.38

**CAS:** 160788-98-7



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-271.67	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-506.30	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	30.04	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	76.17	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.75		Crippen Method
$P_c$	2629.85	kPa	Joback Method
$T_{\text{boil}}$	690.79	K	Joback Method
$T_c$	921.71	K	Joback Method
$T_{\text{fus}}$	398.65	K	Joback Method
$V_c$	0.85	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	591.10	J/mol×K	690.79	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H18O3S/c1-16\(2,3\)13-9-11-14\(12-10-13\)19-20\(17,18\)15-7-5-4-6-8-15/h4-12H,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H18O3S/c1-16(2,3)13-9-11-14(12-10-13)19-20(17,18)15-7-5-4-6-8-15/h4-12H,1-3H3)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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