Benzenesulfonic acid, 4-methyl-, butyl ester

Other names:	p-Toluenesulfonic acid, butyl ester
	Butyl p-methylbenzenesulfonate
	Butyl p-toluenesulfonate
	Butyl tosylate
	Butyl para-toluenesulfonate
	n-Butyl p-toluenesulfonate
	Butyl ester of 4-toluenesulfonic acid
	Butyl 4-methylbenzenesulfonate
	NSC 6190
	butyl toluene-4-sulphonate
Inchi:	InChI=1S/C11H16O3S/c1-3-4-9-14-15(12,13)11-7-5-10(2)6-8-11/h5-8H,3-4,9H2,1-2H3
InchiKey:	QYJXDIUNDMRLAO-UHFFFAOYSA-N
Formula:	C11H16O3S
SMILES:	CCCCOS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	228.31
CAS:	778-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-429.02	kJ/mol	Joback Method
hf	-630.88	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.500		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	552.94	K	Joback Method
tc	748.21	K	Joback Method
tf	313.46	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.73	J/mol×K	552.94	Joback Method
cpg	424.05	J/mol×K	585.48	Joback Method
cpg	438.61	J/mol×K	618.03	Joback Method
cpg	452.42	J/mol×K	650.57	Joback Method
cpg	465.46	J/mol×K	683.12	Joback Method
cpg	477.75	J/mol×K	715.66	Joback Method
cpg	489.29	J/mol×K	748.21	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C778289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume