

Benzenesulfonamide, N-butyl-4-methyl-

Other names:	p-Toluenesulfonamide, N-butyl- N-Butyl-p-toluenesulfonamide N-Tosylbutylamine n-Butyl-4-toluenesulfonamide N-n-Butyl-4-toluenesulfonamide N-n-Butyl-p-toluene sulfonamide 4-(N-1-Butyl)toluenesulfonamide n-Butyl-4-methylbenzenesulfonamide NSC 2180 N-butyltoluene-4-sulphonamide
Inchi:	InChI=1S/C11H17NO2S/c1-3-4-9-12-15(13,14)11-7-5-10(2)6-8-11/h5-8,12H,3-4,9H2,1-2
InchiKey:	RQUXYBHREKXNKT-UHFFFAOYSA-N
Formula:	C11H17NO2S
SMILES:	CCCCNS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	227.32
CAS:	1907-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-234.63	kJ/mol	Joback Method
hf	-445.19	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	68.09	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.073		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	580.69	K	Joback Method
tc	778.46	K	Joback Method
tf	343.89	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.05	J/mol×K	580.69	Joback Method
cpg	450.52	J/mol×K	613.65	Joback Method
cpg	465.13	J/mol×K	646.61	Joback Method
cpg	478.89	J/mol×K	679.58	Joback Method
cpg	491.82	J/mol×K	712.54	Joback Method
cpg	503.92	J/mol×K	745.50	Joback Method
cpg	515.23	J/mol×K	778.46	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=C1907659&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
mccol:	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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