Toluenesulfonamide, n-ethyl-, (mixture of o-and p-)

Inchi: InChI=1S/2C9H13NO2S/c1-3-10-13(11,12)9-6-4-8(2)5-7-9;1-3-10-13(11,12)9-7-5-4-6-8(9

InchiKey: IDLSDSKPHLCUTN-UHFFFAOYSA-N

Formula: C18H26N2O4S2

SMILES: CCNS(=O)(=O)c1ccc(C)cc1.CCNS(=O)(=O)c1ccccc1C

Mol. weight [g/mol]: 398.54

Physical Properties

Property code	Value	Unit	Source
gf	-556.82	kJ/mol	Joback Method
hf	-876.11	kJ/mol	Joback Method
hfus	59.27	kJ/mol	Joback Method
hvap	111.97	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	2.586		Crippen Method
mcvol	303.960	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
tb	871.86	K	Joback Method
tc	1088.39	K	Joback Method
tf	520.20	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.72	J/mol×K	871.86	Joback Method
cpg	921.98	J/mol×K	907.95	Joback Method
cpg	934.26	J/mol×K	944.04	Joback Method
cpg	944.54	J/mol×K	980.12	Joback Method
cpg	952.78	J/mol×K	1016.21	Joback Method
cpg	958.94	J/mol×K	1052.30	Joback Method
cpg	963.00	J/mol×K	1088.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009652&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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