Benzene, (ethylsulfonyl)-

Other names:	Sulfone, ethyl phenyl
	Ethyl phenyl sulfone
	Phenyl ethyl sulfone
	(ethylsulphonyl)benzene
Inchi:	InChI=1S/C8H10O2S/c1-2-11(9,10)8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	VBQUDDWATQWCPP-UHFFFAOYSA-N
Formula:	C8H10O2S
SMILES:	CCS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	170.23
CAS:	599-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-339.65	kJ/mol	Joback Method
hf	-425.27	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
log10ws	-1.58		Crippen Method
logp	1.480		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
tb	456.90	K	Joback Method
tc	660.54	K	Joback Method
tf	244.90	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	456.90	Joback Method
cpg	262.27	J/mol×K	490.84	Joback Method
cpg	274.88	J/mol×K	524.78	Joback Method

cpg	286.79	J/mol×K	558.72	Joback Method
cpg	298.00	J/mol×K	592.66	Joback Method
cpg	308.54	J/mol×K	626.60	Joback Method
cpg	318.41	J/mol×K	660.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C599702&Units=SI

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
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