Benzene, (propylsulfonyl)-

Inchi: InChI=1S/C9H12O2S/c1-2-8-12(10,11)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey: OKHILJWKJWMSEP-UHFFFAOYSA-N
Formula: C9H12O2S
SMILES: CCCS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 184.25
CAS: 13596-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-331.23	kJ/mol	Joback Method
hf	-445.91	kJ/mol	Joback Method
hfus	24.48	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
ie	9.21 ± 0.03	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.870		Crippen Method
mcvol	142.000	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	479.78	K	Joback Method
tc	680.81	K	Joback Method
tf	256.17	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.47	J/mol×K	479.78	Joback Method
cpg	305.82	J/mol×K	513.29	Joback Method
cpg	319.40	J/mol×K	546.79	Joback Method
cpg	332.22	J/mol×K	580.30	Joback Method
cpg	344.30	J/mol×K	613.80	Joback Method
cpg	355.66	J/mol×K	647.31	Joback Method
cpg	366.30	J/mol×K	680.81	Joback Method

Sources

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=C13596753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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