Phenyl propargyl sulfone

Inchi: InChI=1S/C9H8O2S/c1-2-8-12(10,11)9-6-4-3-5-7-9/h1,3-7H,8H2
InchiKey: XRZMPJGMAIXQRM-UHFFFAOYSA-N
Formula: C9H8O2S
SMILES: C#CCS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 180.22
CAS: 2525-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-108.16	kJ/mol	Joback Method
hf	-154.01	kJ/mol	Joback Method
hfus	27.46	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.094		Crippen Method
mcvol	133.400	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	469.90	K	Joback Method
tc	686.02	K	Joback Method
tf	303.14	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.55	J/mol×K	469.90	Joback Method
cpg	272.42	J/mol×K	505.92	Joback Method
cpg	284.48	J/mol×K	541.94	Joback Method
cpg	295.76	J/mol×K	577.96	Joback Method
cpg	306.27	J/mol×K	613.98	Joback Method
cpg	316.04	J/mol×K	650.00	Joback Method
cpg	325.09	J/mol×K	686.02	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=C2525408&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
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