

Phenyl prop-1-ynyl sulphone

Inchi:	InChI=1S/C9H8O2S/c1-2-8-12(10,11)9-6-4-3-5-7-9/h3-7H,1H3
InchiKey:	LYYXDHMLCDVGGI-UHFFFAOYSA-N
Formula:	C9H8O2S
SMILES:	CC#CS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	180.22
CAS:	2525-41-9

Physical Properties

Property code	Value	Unit	Source
chs	-5235.10 ± 4.10	kJ/mol	NIST Webbook
gf	-128.43	kJ/mol	Joback Method
hf	43.50 ± 5.00	kJ/mol	NIST Webbook
hfs	-51.90 ± 4.20	kJ/mol	NIST Webbook
hfus	27.61	kJ/mol	Joback Method
hsub	95.00 ± 3.00	kJ/mol	NIST Webbook
hvap	58.69	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.441		Crippen Method
mcvol	133.400	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	488.78	K	Joback Method
tc	717.80	K	Joback Method
tf	362.27	K	Joback Method
vc	0.519	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.30	J/mol×K	488.78	Joback Method
cpg	272.58	J/mol×K	526.95	Joback Method
cpg	285.04	J/mol×K	565.12	Joback Method
cpg	296.70	J/mol×K	603.29	Joback Method
cpg	307.56	J/mol×K	641.46	Joback Method
cpg	317.65	J/mol×K	679.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2525419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

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