1-Methyl-4-(1-propynyl-sulphonyl)benzene

Inchi: InChI=1S/C10H10O2S/c1-3-8-13(11,12)10-6-4-9(2)5-7-10/h4-7H,1-2H3
InchiKey: VOSCFWYOCZJNQB-UHFFFAOYSA-N
Formula: C10H10O2S
SMILES: CC#CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 194.25
CAS: 14027-53-3

Physical Properties

Property code	Value	Unit	Source
chs	-5873.30 ± 3.20	kJ/mol	NIST Webbook
gf	-129.64	kJ/mol	Joback Method
hf	10.40 ± 4.20	kJ/mol	NIST Webbook
hfs	-93.00 ± 3.30	kJ/mol	NIST Webbook
hfus	29.81	kJ/mol	Joback Method
hsub	103.00 ± 3.00	kJ/mol	NIST Webbook
hvap	61.58	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	1.750		Crippen Method
mcvol	147.490	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	516.64	K	Joback Method
tc	742.91	K	Joback Method
tf	386.06	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.39	J/mol×K	516.64	Joback Method
cpg	316.36	J/mol×K	554.35	Joback Method
cpg	329.50	J/mol×K	592.06	Joback Method
cpg	341.84	J/mol×K	629.78	Joback Method
cpg	353.39	J/mol×K	667.49	Joback Method
cpg	364.14	J/mol×K	705.20	Joback Method

cpg	374.10	J/mol×K	742.91	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=C14027533&Units=SI

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