1-Methyl-4-(2-propynyl-sulphonyl)benzene

Inchi: InChI=1S/C10H10O2S/c1-3-8-13(11,12)10-6-4-9(2)5-7-10/h1,4-7H,8H2,2H3
InchiKey: ZKABKQMDZXMAMW-UHFFFAOYSA-N
Formula: C10H10O2S
SMILES: C#CCS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 194.25
CAS: 16192-07-7

Physical Properties

Property code	Value	Unit	Source
chs	-5859.70 ± 3.10	kJ/mol	NIST Webbook
gf	-109.37	kJ/mol	Joback Method
hf	0.80 ± 4.20	kJ/mol	NIST Webbook
hfs	-106.60 ± 3.30	kJ/mol	NIST Webbook
hfus	29.66	kJ/mol	Joback Method
hsub	106.00 ± 3.00	kJ/mol	NIST Webbook
hvap	59.28	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.402		Crippen Method
mcvol	147.490	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	497.76	K	Joback Method
tc	711.87	K	Joback Method
tf	326.93	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.17	J/mol×K	497.76	Joback Method
cpg	315.67	J/mol×K	533.45	Joback Method
cpg	328.37	J/mol×K	569.13	Joback Method
cpg	340.29	J/mol×K	604.82	Joback Method
cpg	351.45	J/mol×K	640.50	Joback Method
cpg	361.86	J/mol×K	676.19	Joback Method

cpg	371.54	J/mol×K	711.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16192077&Units=SI
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

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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