1-Methyl-4-(2-methyl-1-propenylsulphonyl)-benze

Inchi: InChI=1S/C11H14O2S/c1-9(2)8-14(12,13)11-6-4-10(3)5-7-11/h4-8H,1-3H3
InchiKey: MRTWSQJEIUUJDE-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: CC(C)=CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 210.29
CAS: 16192-03-3

Physical Properties

Property code	Value	Unit	Source
chs	-6589.80 ± 1.50	kJ/mol	NIST Webbook
gf	-252.35	kJ/mol	Joback Method
hf	-240.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-341.70 ± 1.10	kJ/mol	NIST Webbook
hfus	28.17	kJ/mol	Joback Method
hsub	102.00 ± 2.00	kJ/mol	NIST Webbook
hvap	61.69	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.692		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	534.56	K	Joback Method
tc	744.10	K	Joback Method
tf	272.19	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.37	J/mol×K	534.56	Joback Method
cpg	379.86	J/mol×K	569.48	Joback Method
cpg	394.44	J/mol×K	604.41	Joback Method
cpg	408.12	J/mol×K	639.33	Joback Method
cpg	420.93	J/mol×K	674.25	Joback Method
cpg	432.90	J/mol×K	709.18	Joback Method

cpg	444.07	J/mol×K	744.10	Joback Method

Sources

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=C16192033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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