

(E)-1-Methyl-4-(1-propenyl-sulphonyl)-benzene

Inchi:	InChI=1S/C10H12O2S/c1-3-8-13(11,12)10-6-4-9(2)5-7-10/h3-8H,1-2H3/b8-3+
InchiKey:	BWSQJQVNZGJZDB-FPYGCLRLSA-N
Formula:	C10H12O2S
SMILES:	CC=CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	196.27
CAS:	32228-15-2

Physical Properties

Property code	Value	Unit	Source
chs	-5959.70 ± 1.50	kJ/mol	NIST Webbook
gf	-252.22	kJ/mol	Joback Method
hf	-209.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-292.30 ± 1.70	kJ/mol	NIST Webbook
hfus	26.89	kJ/mol	Joback Method
hsub	84.00 ± 2.00	kJ/mol	NIST Webbook
hvap	59.39	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.302		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	511.80	K	Joback Method
tc	720.70	K	Joback Method
tf	274.88	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.79	J/mol×K	511.80	Joback Method
cpg	333.24	J/mol×K	546.62	Joback Method
cpg	346.84	J/mol×K	581.43	Joback Method
cpg	359.61	J/mol×K	616.25	Joback Method
cpg	371.57	J/mol×K	651.07	Joback Method
cpg	382.76	J/mol×K	685.89	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=C32228152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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