

(Z)-1-Methyl-4-(2-phenylethenyl)sulphonylbenzene

Inchi:	InChI=1S/C15H14O2S/c1-13-7-9-15(10-8-13)18(16,17)12-11-14-5-3-2-4-6-14/h2-12H,1H
InchiKey:	PIALZYNUNCIZLT-QXMHVHEDSA-N
Formula:	C15H14O2S
SMILES:	<chem>Cc1ccc(S(=O)(=O)C=Cc2ccccc2)cc1</chem>
Mol. weight [g/mol]:	258.33
CAS:	54897-33-5

Physical Properties

Property code	Value	Unit	Source
chs	-8329.50 ± 3.30	kJ/mol	NIST Webbook
gf	-97.71	kJ/mol	Joback Method
hf	-59.80 ± 5.00	kJ/mol	NIST Webbook
hfs	-176.00 ± 3.40	kJ/mol	NIST Webbook
hfus	33.88	kJ/mol	Joback Method
hsub	116.00 ± 2.00	kJ/mol	NIST Webbook
hvap	72.79	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.440		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	652.88	K	Joback Method
tc	887.85	K	Joback Method
tf	357.65	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.73	J/molxK	652.88	Joback Method
cpg	503.28	J/molxK	692.04	Joback Method
cpg	518.48	J/molxK	731.20	Joback Method
cpg	532.40	J/molxK	770.36	Joback Method
cpg	545.12	J/molxK	809.52	Joback Method
cpg	556.68	J/molxK	848.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54897335&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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