P-chlorobenzene sulfonic acid, acetylene hydrazide

Inchi: InChI=1S/C14H12Cl2N4O4S2/c15-11-1-5-13(6-2-11)25(21,22)19-17-9-10-18-20-26(23,2

InchiKey: USRRQFPRMVOFJJ-BEQMOXJMSA-N

Formula: C14H12Cl2N4O4S2

SMILES: O=S(=O)(NN=CC=NNS(=O)(=O)c1ccc(Cl)cc1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 435.31

CAS: 116465-37-3

Physical Properties

Property code	Value	Unit	Source
hf	-548.97	kJ/mol	Joback Method
hvap	118.17	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	2.222		Crippen Method
mcvol	272.580	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	1007.16	K	Joback Method
tc	1255.89	K	Joback Method

Sources

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=C116465373&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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