Benzene, 1-chloro-3-(phenylthio)-

Inchi: InChI=1S/C12H9ClS/c13-10-5-4-8-12(9-10)14-11-6-2-1-3-7-11/h1-9H
InchiKey: YNJLAXHIFOICPE-UHFFFAOYSA-N
Formula: C12H9ClS
SMILES: Clc1cccc(Sc2ccccc2)c1
Mol. weight [g/mol]: 220.72
CAS: 38700-88-8

Physical Properties

Property code	Value	Unit	Source
gf	286.54	kJ/mol	Joback Method
hf	196.71	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	58.72	kJ/mol	Joback Method
ie	8.16	eV	NIST Webbook
log10ws	-4.57		Crippen Method
logp	4.491		Crippen Method
mcvol	161.010	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	638.51	K	Joback Method
tc	913.62	K	Joback Method
tf	354.68	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.03	J/mol×K	638.51	Joback Method
cpg	367.27	J/mol×K	684.36	Joback Method
cpg	380.17	J/mol×K	730.21	Joback Method
cpg	391.81	J/mol×K	776.06	Joback Method
cpg	402.27	J/mol×K	821.91	Joback Method
cpg	411.63	J/mol×K	867.76	Joback Method
cpg	419.97	J/mol×K	913.62	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=C38700888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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