2'-Chlorobenzenesulfonanilide

Other names: N-(2-chlorophenyl)benzene sulfonamide
Inchi: InChI=1S/C12H10ClNO2S/c13-11-8-4-5-9-12(11)14-17(15,16)10-6-2-1-3-7-10/h1-9,14H
InchiKey: KMSWCQQQRKBBAH-UHFFFAOYSA-N
Formula: C12H10ClNO2S
SMILES: O=S(=O)(Nc1ccccc1Cl)c1ccccc1
Mol. weight [g/mol]: 267.73
CAS: 21226-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-125.73	kJ/mol	Joback Method
hf	-245.04	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.141		Crippen Method
mcvol	182.730	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	667.68	K	Joback Method
tc	907.90	K	Joback Method
tf	411.50	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.92	J/mol×K	667.68	Joback Method
cpg	447.59	J/mol×K	707.72	Joback Method
cpg	460.02	J/mol×K	747.75	Joback Method
cpg	471.27	J/mol×K	787.79	Joback Method
cpg	481.36	J/mol×K	827.83	Joback Method
cpg	490.35	J/mol×K	867.86	Joback Method
cpg	498.27	J/mol×K	907.90	Joback Method
hfust	33.50	kJ/mol	398.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21226302&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

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
hfust:	Enthalpy of fusion at a given temperature
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