

Benzenesulfonanilide, 4'-chloro-

Other names:	N-(4-chlorophenyl)benzene sulfonamide
Inchi:	InChI=1S/C12H10ClNO2S/c13-10-6-8-11(9-7-10)14-17(15,16)12-4-2-1-3-5-12/h1-9,14H
InchiKey:	ANRCRHLXUCJAKV-UHFFFAOYSA-N
Formula:	C12H10ClNO2S
SMILES:	O=S(=O)(Nc1ccc(Cl)cc1)c1ccccc1
Mol. weight [g/mol]:	267.73
CAS:	4750-28-1

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.92	J/molxK	667.68	Joback Method
cpg	447.59	J/molxK	707.72	Joback Method
cpg	460.02	J/molxK	747.75	Joback Method
cpg	471.27	J/molxK	787.79	Joback Method
cpg	481.36	J/molxK	827.83	Joback Method
cpg	490.35	J/molxK	867.86	Joback Method
cpg	498.27	J/molxK	907.90	Joback Method
hfust	25.80	kJ/mol	394.60	NIST Webbook

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=C4750281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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