4'-CHLOROBENZENESULFONANILIDE

Other names: N-(4-chlorophenyl)benzene sulfonamide
N-(4-chlorophenyl)benzenesulfonamide
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]: 267.74

Physical Properties

Property code	Value	Unit	Source
hfus	35.20	kJ/mol	Joback Method
hvap	100.02	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.87		Cheméo Relay (1.0)
logp	3.141		Crippen Method
mcvol	182.730	ml/mol	McGowan Method
tf	394.60	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents

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	25.80	kJ/mol	394.60	NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
Cheméo Relay (1.0):	
Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents:	https://www.doi.org/10.1021/je500918t
Octanol/Water Partition Coefficients of Sulfonamides: Experimental Determination and Calculation Using Physicochemical Descriptors:	https://www.doi.org/10.1021/je900189v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4750281&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tf:	Normal melting (fusion) point

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