N-phenylbenzenesulfonamide

Inchi: InChI=1S/C12H11NO2S/c14-16(15,12-9-5-2-6-10-12)13-11-7-3-1-4-8-11/h1-10,13H
InchiKey: XAUGWFWQVYXATQ-UHFFFAOYSA-N
Formula: C12H11NO2S
SMILES: O=S(=O)(Nc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 233.29

Physical Properties

Property code	Value	Unit	Source
gf	-104.17	kJ/mol	Joback Method
hf	-217.83	kJ/mol	Joback Method
hfus	23.50 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	71.93	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.487		Crippen Method
mcvol	170.490	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	625.27	K	Joback Method
tc	861.65	K	Joback Method
tf	383.50 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.45	J/mol×K	625.27	Joback Method
cpg	424.74	J/mol×K	664.67	Joback Method
cpg	438.74	J/mol×K	704.06	Joback Method
cpg	451.49	J/mol×K	743.46	Joback Method
cpg	463.06	J/mol×K	782.86	Joback Method

cpg	473.47	J/mol×K	822.26	Joback Method
cpg	482.79	J/mol×K	861.65	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents:	https://www.doi.org/10.1021/je500918t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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