N-METHYL-N-PHENYLBENZENESULFONAMIDE

Other names: Benzenesulfonanilide, N-methyl-
N-Methylbenzenesulfonanilide
Inchi: InChI=1S/C13H13NO2S/c1-14(12-8-4-2-5-9-12)17(15,16)13-10-6-3-7-11-13/h2-11H,1H3
InchiKey: KRXAPUFKQQWAGK-UHFFFAOYSA-N
Formula: C13H13NO2S
SMILES: CN(c1ccccc1)S(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 247.32

Physical Properties

Property code	Value	Unit	Source
af	0.5595		Cheméo Relay (1.0)
gf	-74.36	kJ/mol	Joback Method
hf	-85.90	kJ/mol	Cheméo Relay (1.0)
hfus	31.91	kJ/mol	Joback Method
hvap	89.75	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-3.87		Cheméo Relay (1.0)
logp	2.512		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	636.07	K	Cheméo Relay (1.0)
tc	914.64	K	Cheméo Relay (1.0)
tf	381.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.78	J/mol×K	610.42	Joback Method
cpg	461.67	J/mol×K	648.71	Joback Method
cpg	477.19	J/mol×K	686.99	Joback Method
cpg	491.40	J/mol×K	725.28	Joback Method
cpg	504.37	J/mol×K	763.57	Joback Method
cpg	516.14	J/mol×K	801.86	Joback Method
cpg	526.79	J/mol×K	840.14	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90108&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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