N,n-dimethyl-4-nitro-3-phenylsulfonylaniline

Inchi: InChI=1S/C14H14N2O4S/c1-15(2)11-8-9-13(16(17)18)14(10-11)21(19,20)12-6-4-3-5-7-1
InchiKey: KUYCVJFSENOEML-UHFFFAOYSA-N
Formula: C14H14N2O4S
SMILES: CN(C)c1ccc([N+](=O)[O-])c(S(=O)(=O)c2ccccc2)c1
Mol. weight [g/mol]: 306.34
CAS: 19770-95-7

Physical Properties

Property code	Value	Unit	Source
gf	-49.65	kJ/mol	Joback Method
hf	-278.75	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	89.90	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.494		Crippen Method
mcvol	216.090	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	795.10	K	Joback Method
tc	1041.09	K	Joback Method
tf	540.06	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.98	J/mol×K	795.10	Joback Method
cpg	612.23	J/mol×K	836.10	Joback Method
cpg	624.10	J/mol×K	877.10	Joback Method
cpg	634.64	J/mol×K	918.09	Joback Method
cpg	643.91	J/mol×K	959.09	Joback Method
cpg	651.98	J/mol×K	1000.09	Joback Method
cpg	658.90	J/mol×K	1041.09	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770957&Units=SI

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