4-Nitro-4'-aminodiphenylsulfone

Other names: 4-(4-Nitrophenylsulfonyl)aniline
Benzenamine, 4-[(4-nitrophenyl)sulfonyl]-
Inchi: InChI=1S/C12H10N2O4S/c13-9-1-5-11(6-2-9)19(17,18)12-7-3-10(4-8-12)14(15)16/h1-8H
InchiKey: DMZVYFFBWHBWMO-UHFFFAOYSA-N
Formula: C12H10N2O4S
SMILES: Nc1ccc(S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 278.28
CAS: 1948-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-110.82	kJ/mol	Joback Method
hf	-271.21	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.010		Crippen Method
mcvol	187.910	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	809.43	K	Joback Method
tc	1073.94	K	Joback Method
tf	568.31	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.76	J/mol×K	809.43	Joback Method
cpg	519.78	J/mol×K	853.51	Joback Method
cpg	529.41	J/mol×K	897.60	Joback Method
cpg	537.71	J/mol×K	941.68	Joback Method
cpg	544.72	J/mol×K	985.77	Joback Method
cpg	550.50	J/mol×K	1029.85	Joback Method
cpg	555.11	J/mol×K	1073.94	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=C1948921&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