4-Nitrodiphenylsulfone

Other names: 4-Nitrophenyl phenyl sulfone
Benzene, 1-nitro-4-(phenylsulfonyl)-
Inchi: InChI=1S/C12H9NO4S/c14-13(15)10-6-8-12(9-7-10)18(16,17)11-4-2-1-3-5-11/h1-9H
InchiKey: OECHJYYZMSUILG-UHFFFAOYSA-N
Formula: C12H9NO4S
SMILES: O=[N+]([O-])c1ccc(S(=O)(=O)c2ccccc2)cc1
Mol. weight [g/mol]: 263.27
CAS: 1146-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-167.64	kJ/mol	Joback Method
hf	-293.53	kJ/mol	Joback Method
hfus	37.27	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.428		Crippen Method
mcvol	177.930	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	731.92	K	Joback Method
tc	992.42	K	Joback Method
tf	472.53	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.12	J/mol×K	731.92	Joback Method
cpg	468.88	J/mol×K	775.34	Joback Method
cpg	480.24	J/mol×K	818.75	Joback Method
cpg	490.25	J/mol×K	862.17	Joback Method
cpg	498.98	J/mol×K	905.59	Joback Method
cpg	506.48	J/mol×K	949.01	Joback Method
cpg	512.80	J/mol×K	992.42	Joback Method

Sources

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=C1146390&Units=SI
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