4-Nitrobenzenesulphonyl chloride

Other names:	Benzenesulfonyl chloride, p-nitro-
	p-Nitrobenzenesulfonyl chloride
	p-Nitrophenylsulfonyl chloride
	4-Nitrobenzenesulfonic acid chloride
	4-Nitrobenzenesulfonyl chloride
	4-Nitrophenylsulfonyl chloride
	Benzenesulfonyl chloride, 4-nitro-
	p-Nitrobenzenesulphonyl chloride
	NSC 13065
Inchi:	InChI=1S/C6H4ClNO4S/c7-13(11,12)6-3-1-5(2-4-6)8(9)10/h1-4H
InchiKey:	JXRGUPLJCCDGKG-UHFFFAOYSA-N
Formula:	C6H4ClNO4S
SMILES:	O=[N+]([O-])c1ccc(S(=O)(=O)Cl)cc1
Mol. weight [g/mol]:	221.62
CAS:	98-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-342.50	kJ/mol	Joback Method
hf	-421.96	kJ/mol	Joback Method
hfus	31.88	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.522		Crippen Method
mcvol	129.390	ml/mol	McGowan Method
pc	5503.26	kPa	Joback Method
tb	605.39	K	Joback Method
tc	852.34	K	Joback Method
tf	408.41	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	273.56	J/mol×K	605.39	Joback Method
cpg	283.06	J/mol×K	646.55	Joback Method
cpg	291.71	J/mol×K	687.71	Joback Method
cpg	299.53	J/mol×K	728.86	Joback Method
cpg	306.53	J/mol×K	770.02	Joback Method
cpg	312.71	J/mol×K	811.18	Joback Method
cpg	318.10	J/mol×K	852.34	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=C98748&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