p-Nitrobenzenesulfonyl 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

Physical Properties

Property code	Value	Unit	Source
hf	-255.25	kJ/mol	Cheméo Relay (1.0)
hfus	31.88	kJ/mol	Joback Method
hvap	89.23	kJ/mol	Cheméo Relay (1.0)
ie	10.48	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	1.522		Crippen Method
mcvol	129.390	ml/mol	McGowan Method
tb	559.54	K	Cheméo Relay (1.0)
tf	421.78	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98748&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point