2-Nitrobenzenesulfonyl fluoride

Other names:	o-Nitrobenzenesulfonyl fluoride
	Benzenesulfonyl fluoride, 2-nitro-
	Benzenesulfonyl fluoride, o-nitro-
	2-nitrobenzenesulphonyl fluoride
Inchi:	InChI=1S/C6H4FNO4S/c7-13(11,12)6-4-2-1-3-5(6)8(9)10/h1-4H
InchiKey:	HSQIQAVSSNKMBM-UHFFFAOYSA-N
Formula:	C6H4FNO4S
SMILES:	O=[N+]([O-])c1ccccc1S(=O)(=O)F
Mol. weight [g/mol]:	205.16
CAS:	433-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-525.38	kJ/mol	Joback Method
hf	-602.33	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	66.30	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.253		Crippen Method
mcvol	118.920	ml/mol	McGowan Method
pc	5438.52	kPa	Joback Method
tb	567.23	K	Joback Method
tc	798.17	K	Joback Method
tf	379.08	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.70	J/mol×K	567.23	Joback Method
cpg	270.58	J/mol×K	605.72	Joback Method
cpg	279.71	J/mol×K	644.21	Joback Method
cpg	288.10	J/mol×K	682.70	Joback Method
cpg	295.74	J/mol×K	721.19	Joback Method

cpg	302.66	J/mol×K	759.68	Joback Method
cpg	308.86	J/mol×K	798.17	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=C433987&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