Methyl 4-nitrophenyl sulfone

Other names:	Sulfone, methyl p-nitrophenyl
	Methyl p-nitrophenyl sulfone
	Benzene, 1-(methylsulfonyl)-4-nitro-
Inchi:	InChI=1S/C7H7NO4S/c1-13(11,12)7-4-2-6(3-5-7)8(9)10/h2-5H,1H3
InchiKey:	XONGBDXIFQIQBN-UHFFFAOYSA-N
Formula:	C7H8NO4S
SMILES:	CS(=O)(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	202.21
CAS:	2976-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-322.15	kJ/mol	Joback Method
hf	-426.86	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	69.34	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	0.998		Crippen Method
mcvol	131.240	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
tb	590.84	K	Joback Method
tc	829.13	K	Joback Method
tf	389.76	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.06	J/mol×K	590.84	Joback Method
cpg	308.50	J/mol×K	630.55	Joback Method
cpg	319.07	J/mol×K	670.27	Joback Method
cpg	328.78	J/mol×K	709.98	Joback Method
cpg	337.62	J/mol×K	749.70	Joback Method
cpg	345.62	J/mol×K	789.41	Joback Method

cpg	352.79	J/mol×K	829.13	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=C2976309&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

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