Benzenesulfonyl chloride, 4-methoxy-

Other names:	Benzenesulfonyl chloride, p-methoxy- p-Anisylsulfonyl chloride p-Methoxybenzenesulfonyl chloride p-Methoxyphenylsulfonyl chloride 4-Methoxybenzenesulfonyl chloride 4-methoxybenzenesulphonyl chloride
Inchi:	InChI=1S/C7H7ClO3S/c1-11-6-2-4-7(5-3-6)12(8,9)10/h2-5H,1H3
InchiKey:	DTJVECUKADWGMO-UHFFFAOYSA-N
Formula:	C7H7ClO3S
SMILES:	COc1ccc(S(=O)(=O)Cl)cc1
Mol. weight [g/mol]:	206.65
CAS:	98-68-0

Physical Properties

Property code	Value	Unit	Source
gf	-474.63	kJ/mol	Joback Method
hf	-564.06	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.623		Crippen Method
mcvol	131.930	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	498.85	K	Joback Method
tc	710.87	K	Joback Method
tf	298.30	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.21	J/mol×K	498.85	Joback Method
cpg	267.10	J/mol×K	534.19	Joback Method
cpg	277.43	J/mol×K	569.52	Joback Method

cpg	287.20	J/mol×K	604.86	Joback Method
cpg	296.39	J/mol×K	640.19	Joback Method
cpg	304.99	J/mol×K	675.53	Joback Method
cpg	312.99	J/mol×K	710.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98680&Units=SI
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

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