Benzenesulfonyl chloride, 4-(trifluoromethoxy)-

Other names: p-(trifluoromethoxy)benzenesulphonyl chloride
Inchi: InChI=1S/C7H4ClF3O3S/c8-15(12,13)6-3-1-5(2-4-6)14-7(9,10)11/h1-4H
InchiKey: UHCDBMIOLNKDHG-UHFFFAOYSA-N
Formula: C7H4ClF3O3S
SMILES: O=S(=O)(Cl)c1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 260.62
CAS: 94108-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-1056.22	kJ/mol	Joback Method
hf	-1161.14	kJ/mol	Joback Method
hfus	26.13	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.513		Crippen Method
mcvol	137.240	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	493.43	K	Joback Method
tc	686.61	K	Joback Method
tf	302.49	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.68	J/mol×K	493.43	Joback Method
cpg	294.86	J/mol×K	525.63	Joback Method
cpg	304.41	J/mol×K	557.82	Joback Method
cpg	313.35	J/mol×K	590.02	Joback Method
cpg	321.68	J/mol×K	622.21	Joback Method
cpg	329.41	J/mol×K	654.41	Joback Method
cpg	336.55	J/mol×K	686.61	Joback Method

Sources

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=C94108562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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