Benzenesulfonyl chloride, 2-(trifluoromethyl)-

Other names: 2-(Chlorosulfonyl)benzenetrifluoride
Inchi: InChI=1S/C7H4ClF3O2S/c8-14(12,13)6-4-2-1-3-5(6)7(9,10)11/h1-4H
InchiKey: ZIZGWNOAHUCACM-UHFFFAOYSA-N
Formula: C7H4ClF3O2S
SMILES: O=S(=O)(Cl)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 244.62
CAS: 776-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-951.22	kJ/mol	Joback Method
hf	-1028.92	kJ/mol	Joback Method
hfus	24.94	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.633		Crippen Method
mcvol	131.370	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	471.01	K	Joback Method
tc	665.42	K	Joback Method
tf	280.26	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.58	J/mol×K	471.01	Joback Method
cpg	273.08	J/mol×K	503.41	Joback Method
cpg	282.88	J/mol×K	535.81	Joback Method
cpg	291.99	J/mol×K	568.21	Joback Method
cpg	300.45	J/mol×K	600.62	Joback Method
cpg	308.27	J/mol×K	633.02	Joback Method
cpg	315.47	J/mol×K	665.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C776045&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

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