4-(Trifluoromethoxy)benzenesulphonyl chloride

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

Physical Properties

Property code	Value	Unit	Source
hfus	26.13	kJ/mol	Joback Method
ie	9.80	eV	Cheméo Relay (1.0)
logp	2.513		Crippen Method
mcvol	137.240	ml/mol	McGowan Method
tb	498.67	K	Cheméo Relay (1.0)

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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94108562&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature