2,5-Dimethoxybenzenesulfonyl chloride

Inchi: InChI=1S/C8H9ClO4S/c1-12-6-3-4-7(13-2)8(5-6)14(9,10)11/h3-5H,1-2H3
InchiKey: SHELADVIRCCTFN-UHFFFAOYSA-N
Formula: C8H9ClO4S
SMILES: COc1ccc(OC)c(S(=O)(=O)Cl)c1
Mol. weight [g/mol]: 236.67
CAS: 1483-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-580.84	kJ/mol	Joback Method
hf	-728.39	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.631		Crippen Method
mcvol	151.890	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	549.13	K	Joback Method
tc	756.92	K	Joback Method
tf	344.32	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.29	J/mol×K	549.13	Joback Method
cpg	332.81	J/mol×K	583.76	Joback Method
cpg	343.81	J/mol×K	618.39	Joback Method
cpg	354.24	J/mol×K	653.02	Joback Method
cpg	364.08	J/mol×K	687.66	Joback Method
cpg	373.30	J/mol×K	722.29	Joback Method
cpg	381.89	J/mol×K	756.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1483289&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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