4-Methyl-1,3-benzenedisulfonyl dichloride

Inchi: InChI=1S/C7H6Cl2O4S2/c1-5-2-3-6(14(8,10)11)4-7(5)15(9,12)13/h2-4H,1H3
InchiKey: CLMMQDZNOXYEBU-UHFFFAOYSA-N
Formula: C7H6Cl2O4S2
SMILES: Cc1ccc(S(=O)(=O)Cl)cc1S(=O)(=O)Cl
Mol. weight [g/mol]: 289.16
CAS: 2767-77-3

Physical Properties

Property code	Value	Unit	Source
gf	-859.73	kJ/mol	Joback Method
hf	-912.40	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Joback Method
hvap	80.82	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.850		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
pc	5462.66	kPa	Joback Method
tb	566.62	K	Joback Method
tc	778.90	K	Joback Method
tf	357.07	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.50	J/mol×K	566.62	Joback Method
cpg	343.05	J/mol×K	602.00	Joback Method
cpg	352.92	J/mol×K	637.38	Joback Method
cpg	362.09	J/mol×K	672.76	Joback Method
cpg	370.54	J/mol×K	708.14	Joback Method
cpg	378.26	J/mol×K	743.52	Joback Method
cpg	385.24	J/mol×K	778.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2767773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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