p-Methylsulfonylbenzyl chloride

Inchi: InChI=1S/C8H9ClO2S/c1-12(10,11)8-4-2-7(6-9)3-5-8/h2-5H,6H2,1H3
InchiKey: LXPRVXKHIXWBJZ-UHFFFAOYSA-N
Formula: C8H9ClO2S
SMILES: CS(=O)(=O)c1ccc(CCl)cc1
Mol. weight [g/mol]: 204.67
CAS: 53606-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-361.21	kJ/mol	Joback Method
hf	-452.48	kJ/mol	Joback Method
hfus	25.70	kJ/mol	Joback Method
hvap	59.36	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.829		Crippen Method
mcvol	140.150	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	499.31	K	Joback Method
tc	710.08	K	Joback Method
tf	287.34	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.01	J/mol×K	499.31	Joback Method
cpg	288.26	J/mol×K	534.44	Joback Method
cpg	299.81	J/mol×K	569.57	Joback Method
cpg	310.68	J/mol×K	604.70	Joback Method
cpg	320.86	J/mol×K	639.83	Joback Method
cpg	330.38	J/mol×K	674.96	Joback Method
cpg	339.23	J/mol×K	710.08	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=C53606067&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