Benzoic acid, 4-[(4-chlorophenyl)sulfonyl]-

Other names: 4-Chloro-4'-carboxydiphenyl sulfone
Inchi: InChI=1S/C13H9ClO4S/c14-10-3-7-12(8-4-10)19(17,18)11-5-1-9(2-6-11)13(15)16/h1-8H
InchiKey: MIVYLPYNSKNBPW-UHFFFAOYSA-N
Formula: C13H9ClO4S
SMILES: O=C(O)c1ccc(S(=O)(=O)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 296.73
CAS: 37940-65-1

Physical Properties

Property code	Value	Unit	Source
gf	-482.07	kJ/mol	Joback Method
hf	-595.43	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	96.85	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.871		Crippen Method
mcvol	194.280	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	791.42	K	Joback Method
tc	1017.05	K	Joback Method
tf	493.38	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.77	J/mol×K	791.42	Joback Method
cpg	501.22	J/mol×K	829.02	Joback Method
cpg	509.67	J/mol×K	866.63	Joback Method
cpg	517.16	J/mol×K	904.23	Joback Method
cpg	523.71	J/mol×K	941.84	Joback Method
cpg	529.36	J/mol×K	979.44	Joback Method
cpg	534.13	J/mol×K	1017.05	Joback Method

Sources

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=C37940651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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