O,o'-sulfonyl dibenzoic acid

Inchi: InChI=1S/C14H10O6S/c15-13(16)9-5-1-3-7-11(9)21(19,20)12-8-4-2-6-10(12)14(17)18/h1
InchiKey: AOFRNZNXMCOXHP-UHFFFAOYSA-N
Formula: C14H10O6S
SMILES: O=C(O)c1ccccc1S(=O)(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 306.29
CAS: 22219-00-7

Physical Properties

Property code	Value	Unit	Source
gf	-727.46	kJ/mol	Joback Method
hf	-865.14	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	118.12	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.916		Crippen Method
mcvol	203.570	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
tb	922.92	K	Joback Method
tc	1142.54	K	Joback Method
tf	585.48	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.27	J/mol×K	922.92	Joback Method
cpg	576.87	J/mol×K	959.52	Joback Method
cpg	582.53	J/mol×K	996.13	Joback Method
cpg	587.29	J/mol×K	1032.73	Joback Method
cpg	591.15	J/mol×K	1069.33	Joback Method
cpg	594.17	J/mol×K	1105.93	Joback Method
cpg	596.35	J/mol×K	1142.54	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=C22219007&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