

4,4'-SULFONYLDIBENZOIC ACID

Other names:	p,p'-Sulfonyl dibenzoic acid
Inchi:	InChI=1S/C14H10O6S/c15-13(16)9-1-5-11(6-2-9)21(19,20)12-7-3-10(4-8-12)14(17)18/h1
InchiKey:	SQJQLYOMPSJVQS-UHFFFAOYSA-N
Formula:	C14H10O6S
SMILES:	O=C(O)c1ccc(S(=O)(=O)c2ccc(C(=O)O)cc2)cc1
Mol. weight [g/mol]:	306.29

Physical Properties

Property code	Value	Unit	Source
af	1.0267		Cheméo Relay (1.0)
gf	-727.46	kJ/mol	Joback Method
hf	-815.75	kJ/mol	Cheméo Relay (1.0)
hfus	42.07	kJ/mol	Joback Method
hvap	166.95	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	1.916		Crippen Method
mcvol	203.570	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
tb	676.56	K	Cheméo Relay (1.0)
tc	1023.39	K	Cheméo Relay (1.0)
tf	573.72	K	Cheméo Relay (1.0)
vc	0.703	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2449356&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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