

M,m'-sulfonyl dibenzoic acid

Inchi:	InChI=1S/C14H10O6S/c15-13(16)9-3-1-5-11(7-9)21(19,20)12-6-2-4-10(8-12)14(17)18/h
InchiKey:	BBECNDJSLQBLJL-UHFFFAOYSA-N
Formula:	C14H10O6S
SMILES:	O=C(O)c1cccc(S(=O)(=O)c2cccc(C(=O)O)c2)c1
Mol. weight [g/mol]:	306.29
CAS:	22452-74-0

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/molxK	922.92	Joback Method
cpg	576.87	J/molxK	959.52	Joback Method
cpg	582.53	J/molxK	996.13	Joback Method
cpg	587.29	J/molxK	1032.73	Joback Method
cpg	591.15	J/molxK	1069.33	Joback Method
cpg	594.17	J/molxK	1105.93	Joback Method
cpg	596.35	J/molxK	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=C22452740&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

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