2,4-Dimethyldiphenylsulfone

Other names: Sulfone, phenyl, 2,4-xylyl
Inchi: InChI=1S/C14H14O2S/c1-11-8-9-14(12(2)10-11)17(15,16)13-6-4-3-5-7-13/h3-10H,1-2H3
InchiKey: ZCVSDPUSEUOUHQ-UHFFFAOYSA-N
Formula: C14H14O2S
SMILES: Cc1ccc(S(=O)(=O)c2ccccc2)c(C)c1
Mol. weight [g/mol]: 246.32
CAS: 4212-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-195.98	kJ/mol	Joback Method
hf	-335.52	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	71.27	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.136		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	630.82	K	Joback Method
tc	861.63	K	Joback Method
tf	358.00 ± 2.00	K	NIST Webbook
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.66	J/mol×K	630.82	Joback Method
cpg	473.14	J/mol×K	669.29	Joback Method
cpg	488.39	J/mol×K	707.76	Joback Method
cpg	502.46	J/mol×K	746.22	Joback Method
cpg	515.36	J/mol×K	784.69	Joback Method
cpg	527.14	J/mol×K	823.16	Joback Method
cpg	537.83	J/mol×K	861.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4212742&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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