Di-(p-ethylphenyl)sulfone

Inchi: InChI=1S/C16H18O2S/c1-3-13-5-9-15(10-6-13)19(17,18)16-11-7-14(4-2)8-12-16/h5-12H
InchiKey: SYTJCVCXQZUFKK-UHFFFAOYSA-N
Formula: C16H18O2S
SMILES: CCc1ccc(S(=O)(=O)c2ccc(CC)cc2)cc1
Mol. weight [g/mol]: 274.38
CAS: 66294-51-7

Physical Properties

Property code	Value	Unit	Source
gf	-179.14	kJ/mol	Joback Method
hf	-376.80	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	75.72	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.644		Crippen Method
mcvol	216.870	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	676.58	K	Joback Method
tc	898.88	K	Joback Method
tf	386.52	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.42	J/mol×K	676.58	Joback Method
cpg	577.63	J/mol×K	713.63	Joback Method
cpg	593.58	J/mol×K	750.68	Joback Method
cpg	608.30	J/mol×K	787.73	Joback Method
cpg	621.84	J/mol×K	824.78	Joback Method
cpg	634.23	J/mol×K	861.83	Joback Method
cpg	645.50	J/mol×K	898.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66294517&Units=SI

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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