2,4,4'-Trimethyldiphenylsulphone

Other names: 2,4-dimethyl 4-methylphenyl sulfone
Inchi: InChI=1S/C15H16O2S/c1-11-4-7-14(8-5-11)18(16,17)15-9-6-12(2)13(3)10-15/h4-10H,1-3
InchiKey: VBDKBFUQKJPPLF-UHFFFAOYSA-N
Formula: C15H16O2S
SMILES: Cc1ccc(S(=O)(=O)c2ccc(C)c(C)c2)cc1
Mol. weight [g/mol]: 260.35
CAS: 13249-97-3

Physical Properties

Property code	Value	Unit	Source
gf	-197.19	kJ/mol	Joback Method
hf	-367.63	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	74.16	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.445		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	658.68	K	Joback Method
tc	885.95	K	Joback Method
tf	387.77	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.27	J/mol×K	658.68	Joback Method
cpg	523.95	J/mol×K	696.56	Joback Method
cpg	539.42	J/mol×K	734.44	Joback Method
cpg	553.71	J/mol×K	772.31	Joback Method
cpg	566.85	J/mol×K	810.19	Joback Method
cpg	578.86	J/mol×K	848.07	Joback Method
cpg	589.77	J/mol×K	885.95	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=C13249973&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