

Diphenylsulfone, 2,2',4,4',6,6'-hexamethyl-

Other names:	Benzene, 1,1'-sulfonylbis(2,4,6-trimethyl- Bis(2,4,6-trimethylphenyl) sulfone Mesityl sulfone 1,1'-Sulfonylbis(2,4,6-trimethylbenzene) 2,2',4,4',6,6'-Hexamethyldiphenyl sulfone
Inchi:	InChI=1S/C18H22O2S/c1-11-7-13(3)17(14(4)8-11)21(19,20)18-15(5)9-12(2)10-16(18)6/h
InchiKey:	QKCBXXUTOURERT-UHFFFAOYSA-N
Formula:	C18H22O2S
SMILES:	Cc1cc(C)c(S(=O)(=O)c2c(C)cc(C)cc2C)c(C)c1
Mol. weight [g/mol]:	302.43
CAS:	3112-79-6

Physical Properties

Property code	Value	Unit	Source
gf	-200.82	kJ/mol	Joback Method
hf	-463.96	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	82.82	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.370		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
tb	742.26	K	Joback Method
tc	960.70	K	Joback Method
tf	459.14	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.67	J/mol×K	742.26	Joback Method
cpg	683.71	J/mol×K	778.67	Joback Method
cpg	699.55	J/mol×K	815.07	Joback Method
cpg	714.21	J/mol×K	851.48	Joback Method

cpg	727.68	J/mol×K	887.89	Joback Method
cpg	739.99	J/mol×K	924.30	Joback Method
cpg	751.14	J/mol×K	960.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3112796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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