

2,4,6-TRIMETHYLDIPHENYLSULPHONE

Other names:	Benzene, 1,3,5-trimethyl-2-(phenylsulfonyl)- Mesityl phenyl sulfone Phenyl 2,4,6-trimethylphenyl sulfone Sulfone, mesityl phenyl 2,4,6-Trimethylphenyl phenyl sulfone
Inchi:	InChI=1S/C15H16O2S/c1-11-9-12(2)15(13(3)10-11)18(16,17)14-7-5-4-6-8-14/h4-10H,1-3
InchiKey:	KASDQDYPCNMNLM-UHFFFAOYSA-N
Formula:	C15H16O2S
SMILES:	Cc1cc(C)c(S(=O)(=O)c2ccccc2)c(C)c1
Mol. weight [g/mol]:	260.36

Physical Properties

Property code	Value	Unit	Source
hf	-184.88	kJ/mol	Cheméo Relay (1.0)
hfus	32.90	kJ/mol	Joback Method
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-4.77		Cheméo Relay (1.0)
logp	3.445		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
tf	346.00 ± 2.00	K	NIST Webbook

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3112821&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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