2,5-di-tert-Butyl-1,4-dimethoxybenzene

Other names:	1,4-di-t-Butyl-2,5-dimethoxybenzene
	1,4-di-tert-Butyl-2,5-dimethoxybenzene
	Benzene, 1,4-bis(1,1-dimethylethyl)-2,5-dimethoxy-
Inchi:	InChI=1S/C16H26O2/c1-15(2,3)11-9-14(18-8)12(16(4,5)6)10-13(11)17-7/h9-10H,1-8H3
InchiKey:	ATGCJUULFWEWPY-UHFFFAOYSA-N
Formula:	C16H26O2
SMILES:	COc1cc(C(C)(C)C)c(OC)cc1C(C)(C)C
Mol. weight [g/mol]:	250.38
CAS:	7323-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.96	kJ/mol	Joback Method
hf	-453.39	kJ/mol	Joback Method
hfus	17.62	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.299		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
tb	645.48	K	Joback Method
tc	855.22	K	Joback Method
tf	383.36	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.30	J/mol×K	645.48	Joback Method
cpg	694.51	J/mol×K	820.26	Joback Method
cpg	679.57	J/mol×K	785.30	Joback Method
cpg	663.61	J/mol×K	750.35	Joback Method
cpg	646.61	J/mol×K	715.39	Joback Method
cpg	628.52	J/mol×K	680.44	Joback Method

cpg	708.50	J/mol×K	855.22	Joback Method
dvisc	0.0000682	Pa×s	645.48	Joback Method
dvisc	0.0000896	Pa×s	601.79	Joback Method
dvisc	0.0001227	Pa×s	558.11	Joback Method
dvisc	0.0001774	Pa×s	514.42	Joback Method
dvisc	0.0002746	Pa×s	470.73	Joback Method
dvisc	0.0004649	Pa×s	427.05	Joback Method
dvisc	0.0008872	Pa×s	383.36	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=C7323639&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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