4,6-di-tert-Butyl-m-cresol

Other names:	2,4-Di-t-butyl-5-methylphenol
	2,4-Di-tert-butyl-5-methylphenol
	4,6-Di-t-butyl-m-cresol
	Dbmc
	Phenol, 2,4-bis(1,1-dimethylethyl)-5-methyl-
	m-Cresol, 4,6-di-tert-butyl-
Inchi:	InChI=1S/C15H24O/c1-10-8-13(16)12(15(5,6)7)9-11(10)14(2,3)4/h8-9,16H,1-7H3
InchiKey:	WYSSJDOPILWQDC-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	Cc1cc(O)c(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]:	220.35
CAS:	497-39-2

Physical Properties

Property code	Value	Unit	Source
gf	19.63	kJ/mol	Joback Method
hf	-334.15	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	63.01	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.296		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
tb	653.40	K	Joback Method
tc	880.13	K	Joback Method
tf	426.83	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.63	J/mol×K	880.13	Joback Method
cpg	641.37	J/mol×K	842.35	Joback Method
cpg	627.45	J/mol×K	804.56	Joback Method

cpg	612.75	J/mol×K	766.77	Joback Method
cpg	597.12	J/mol×K	728.98	Joback Method
cpg	580.43	J/mol×K	691.19	Joback Method
cpg	562.55	J/mol×K	653.40	Joback Method
dvisc	0.0006069	Pa×s	426.83	Joback Method
dvisc	0.0000139	Pa×s	653.40	Joback Method
dvisc	0.0000215	Pa×s	615.64	Joback Method
dvisc	0.0000352	Pa×s	577.88	Joback Method
dvisc	0.0000618	Pa×s	540.12	Joback Method
dvisc	0.0001181	Pa×s	502.35	Joback Method
dvisc	0.0002505	Pa×s	464.59	Joback Method
hvapt	67.00	kJ/mol	465.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47505e+01
Coeff. B	-4.75306e+03
Coeff. C	-9.54820e+01
Temperature range (K), min.	424.12
Temperature range (K), max.	599.04

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C497392&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume