Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)-

Other names:	4-tert-Octyl-o-Cresol
	o-Cresol, 4-(1,1,3,3-tetramethylbutyl)-
	2-Methyl-4-tert-octylphenol
	4-(1,1,3,3-Tetramethylbutyl)-o-cresol
	2-Methyl-4-(1,1,3,3-tetramethylbutyl)phenol
Inchi:	InChI=1S/C15H24O/c1-11-9-12(7-8-13(11)16)15(5,6)10-14(2,3)4/h7-9,16H,10H2,1-6H3
InchiKey:	DYKCNMUCTREDMF-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	Cc1cc(C(C)(C)CC(C)(C)C)ccc1O
Mol. weight [g/mol]:	220.35
CAS:	2219-84-3

Physical Properties

Property code	Value	Unit	Source
gf	29.26	kJ/mol	Joback Method
hf	-322.68	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.414		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	648.42	K	Joback Method
tc	874.26	K	Joback Method
tf	414.31	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.97	J/mol×K	648.42	Joback Method
cpg	642.42	J/mol×K	836.62	Joback Method
cpg	628.46	J/mol×K	798.98	Joback Method
cpg	613.68	J/mol×K	761.34	Joback Method

cpg	597.93	J/mol×K	723.70	Joback Method
cpg	581.07	J/mol×K	686.06	Joback Method
cpg	655.71	J/mol×K	874.26	Joback Method
dvisc	0.0000145	Pa×s	648.42	Joback Method
dvisc	0.0000230	Pa×s	609.40	Joback Method
dvisc	0.0000390	Pa×s	570.38	Joback Method
dvisc	0.0000714	Pa×s	531.37	Joback Method
dvisc	0.0001440	Pa×s	492.35	Joback Method
dvisc	0.0003273	Pa×s	453.33	Joback Method
dvisc	0.0008688	Pa×s	414.31	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2219843&Units=SI
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

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