Phenol, 2,4-bis(1,1-dimethylpropyl)-

Other names:	2,4-Bis(1,1-dimethylpropyl)phenol
	2,4-Di-tert-amylphenol
	2,4-Di-tert-pentylphenol
	2,4-di-t-Pentylphenol
	2,4-di-tert-Pentylphenyl
	Di-tert-amylphenol
	Phenol, 2,4-di-tert-pentyl-
	Prodox 156
Inchi:	InChI=1S/C16H26O/c1-7-15(3,4)12-9-10-14(17)13(11-12)16(5,6)8-2/h9-11,17H,7-8H2,1-
InchiKey:	WMVJWKURWRGJCI-UHFFFAOYSA-N
Formula:	C16H26O
SMILES:	CCC(C)(C)c1ccc(O)c(C(C)(C)CC)c1
Mol. weight [g/mol]:	234.38
CAS:	120-95-6

Physical Properties

Property code	Value	Unit	Source
gf	37.68	kJ/mol	Joback Method
hf	-343.32	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	64.57	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.767		Crippen Method
mcvol	218.410	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
tb	671.30	K	Joback Method
tc	893.07	K	Joback Method
tf	425.58	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.08	J/mol×K	671.30	Joback Method

cpg	634.47	J/mol×K	708.26	Joback Method
cpg	651.66	J/mol×K	745.22	Joback Method
cpg	667.78	J/mol×K	782.18	Joback Method
cpg	682.98	J/mol×K	819.14	Joback Method
cpg	697.39	J/mol×K	856.11	Joback Method
cpg	711.15	J/mol×K	893.07	Joback Method
dvisc	0.0006998	Pa×s	425.58	Joback Method
dvisc	0.0002604	Pa×s	466.53	Joback Method
dvisc	0.0001136	Pa×s	507.49	Joback Method
dvisc	0.0000561	Pa×s	548.44	Joback Method
dvisc	0.0000306	Pa×s	589.39	Joback Method
dvisc	0.0000180	Pa×s	630.35	Joback Method
dvisc	0.0000113	Pa×s	671.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34889e+01
Coeff. B	-4.26955e+03
Coeff. C	-9.27020e+01
Temperature range (K), min.	416.12
Temperature range (K), max.	614.81

Sources

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=C120956&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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume