4-tert-octylphenol

Other names:	4-(1,1,3,3-Tetramethylbutyl)phenol
	Phenol, 4-(1,1,3,3-tetramethylbutyl)-
	Phenol, p-(1,1,3,3-tetramethylbutyl)-
	Phenol, p-(tert-octyl)-
	p-(1',1',3',3'-Tetramethylbutyl)phenol
	p-(1,1,3,3-Tetramethylbutyl)phenol
	p-Terc.oktylfenol
	p-tert-Octylphenol
	para-tert-Octylphenol
Inchi:	InChI=1S/C14H22O/c1-13(2,3)10-14(4,5)11-6-8-12(15)9-7-11/h6-9,15H,10H2,1-5H3
InchiKey:	ISAVYTVYFVQUDY-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)CC(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]:	206.32
CAS:	124765-79-3

Physical Properties

Property code	Value	Unit	Source
hf	-275.99	kJ/mol	Cheméo Relay (1.0)
hfus	17.01	kJ/mol	Joback Method
hsub	97.90 ± 0.90	kJ/mol	NIST Webbook
hvap	75.52	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-4.32		Cheméo Relay (1.0)
logp	4.106		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
tb	567.28	K	Cheméo Relay (1.0)
tf	388.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.49	J/mol×K	620.56	Joback Method
cpg	529.53	J/mol×K	658.78	Joback Method

cpg	546.21	J/mol×K	696.99	Joback Method
cpg	561.68	J/mol×K	735.21	Joback Method
cpg	576.11	J/mol×K	773.42	Joback Method
cpg	589.65	J/mol×K	811.64	Joback Method
cpg	602.44	J/mol×K	849.86	Joback Method
dvisc	0.0016156	Pa×s	390.52	Joback Method
dvisc	0.0005565	Pa×s	428.86	Joback Method
dvisc	0.0002283	Pa×s	467.20	Joback Method
dvisc	0.0001072	Pa×s	505.54	Joback Method
dvisc	0.0000560	Pa×s	543.88	Joback Method
dvisc	0.0000319	Pa×s	582.22	Joback Method
dvisc	0.0000194	Pa×s	620.56	Joback Method
hsubt	96.30 ± 0.90	kJ/mol	324.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62643e+01
Coeff. B	-5.32104e+03
Coeff. C	-9.78310e+01
Temperature range (K), min.	430.88
Temperature range (K), max.	583.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.70048e+02
Coeff. B	-1.61286e+04
Coeff. C	-2.20319e+01
Coeff. D	8.64424e-06
Temperature range (K), min.	358.55
Temperature range (K), max.	765.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124765793&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol888.mol
Cheméo Relay (1.0, beta):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=888
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point