Phenol, 3,5-bis(1,1-dimethylethyl)-

Other names:	3,5-Di-t-butylphenol
	3,5-Di-tert-butylphenol
	3,5-bis(1,1-Dimethylethyl)phenol
	Phenol, 3,5-bis(t-butyl)
	Phenol, 3,5-di-tert-butyl-
Inchi:	InChI=1S/C14H22O/c1-13(2,3)10-7-11(14(4,5)6)9-12(15)8-10/h7-9,15H,1-6H3
InchiKey:	ZDWSNKPLZUXBPE-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)c1cc(O)cc(C(C)(C)C)c1
Mol. weight [g/mol]:	206.32
CAS:	1138-52-9

Physical Properties

Property code	Value	Unit	Source
chs	-8242.00	kJ/mol	NIST Webbook
gf	20.84	kJ/mol	Joback Method
hf	-300.00	kJ/mol	NIST Webbook
hfs	-410.00	kJ/mol	NIST Webbook
hfus	16.62	kJ/mol	Joback Method
hsub	97.70 ± 3.70	kJ/mol	NIST Webbook
hsub	110.00	kJ/mol	NIST Webbook
hsub	110.00	kJ/mol	NIST Webbook
hvap	60.12	kJ/mol	Joback Method
ie	7.90 ± 0.02	eV	NIST Webbook
log10ws	-3.65		Crippen Method
logp	3.987		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
ripol	2310.00		NIST Webbook
ripol	2328.00		NIST Webbook
tb	625.54	K	Joback Method
tc	855.78	K	Joback Method
tf	403.04	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.15	J/mol×K	625.54	Joback Method
cpg	528.92	J/mol×K	663.91	Joback Method
cpg	545.39	J/mol×K	702.29	Joback Method
cpg	560.71	J/mol×K	740.66	Joback Method
cpg	575.03	J/mol×K	779.03	Joback Method
cpg	588.49	J/mol×K	817.41	Joback Method
cpg	601.25	J/mol×K	855.78	Joback Method
dvisc	0.0010791	Pa×s	403.04	Joback Method
dvisc	0.0004121	Pa×s	440.12	Joback Method
dvisc	0.0001828	Pa×s	477.21	Joback Method
dvisc	0.0000911	Pa×s	514.29	Joback Method
dvisc	0.0000499	Pa×s	551.37	Joback Method
dvisc	0.0000295	Pa×s	588.46	Joback Method
dvisc	0.0000185	Pa×s	625.54	Joback Method
hsubt	68.20	kJ/mol	313.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36835e+01
Coeff. B	-4.22655e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	404.00
Temperature range (K), max.	593.33

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1138529&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume