Phenol, 2,6-bis(1,1-dimethylethyl)-

Other names: 2,6-(1,1-Dimethylethyl)phenol
2,6-Bis(1,1-dimethylethyl)phenol
2,6-Bis(t-butyl)phenol
2,6-Bis(tert-butyl)phenol
2,6-DTBP
2,6-Di-tert-butylphenol
2,6-di(1,1-dimethylethyl)phenol
2,6-di-t-Butylphenol
AN 701
Ethanox 701
Ethyl 701
Ethyl AN 701
Hitec 4701
Isonox 103
NSC 49175
Phenol, 2,4-di-tert.-butyl
Phenol, 2,6-bis(t-butyl)
Phenol, 2,6-di-tert-butyl-

Inchi: InChI=1S/C14H22O/c1-13(2,3)10-8-7-9-11(12(10)15)14(4,5)6/h7-9,15H,1-6H3

InchiKey: DKCPKDPYUFEZCP-UHFFFAOYSA-N

Formula: C14H22O

SMILES: CC(C)(C)c1cccc(C(C)(C)C)c1O

Mol. weight [g/mol]: 206.32

CAS: 128-39-2

Physical Properties

Property code	Value	Unit	Source
chs	-8280.00	kJ/mol	NIST Webbook
gf	20.84	kJ/mol	Joback Method
hf	-262.00	kJ/mol	NIST Webbook
hfs	-370.00	kJ/mol	NIST Webbook
hfus	16.62	kJ/mol	Joback Method
hsub	81.50 ± 2.30	kJ/mol	NIST Webbook
hsub	108.00	kJ/mol	NIST Webbook
hsub	110.90	kJ/mol	NIST Webbook
hsub	84.60 ± 0.50	kJ/mol	NIST Webbook
hvap	66.00 ± 0.20	kJ/mol	NIST Webbook

ie	7.70 ± 0.02	eV	NIST Webbook
ie	8.15	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
rinpol	1443.20		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1433.60		NIST Webbook
rinpol	1433.60		NIST Webbook
rinpol	1440.10		NIST Webbook
rinpol	1440.10		NIST Webbook
rinpol	1433.60		NIST Webbook
rinpol	1443.20		NIST Webbook
rinpol	1443.20		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2327.00		NIST Webbook
tb	526.20	K	NIST Webbook
tc	855.78	K	Joback Method
tf	310.50 ± 0.50	K	NIST Webbook
tf	311.00 ± 0.20	K	NIST Webbook
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.49	J/mol×K	817.41	Joback Method
cpg	601.25	J/mol×K	855.78	Joback Method
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
dvisc	0.0000295	Pa×s	588.46	Joback Method
dvisc	0.0000185	Pa×s	625.54	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
hfust	16.57	kJ/mol	310.70	NIST Webbook

hfust	16.57	kJ/mol	310.70	NIST Webbook
hvapt	60.40	kJ/mol	458.00	NIST Webbook
hvapt	63.50 ± 0.20	kJ/mol	340.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35468e+01
Coeff. B	-4.16824e+03
Coeff. C	-8.78810e+01
Temperature range (K), min.	402.25
Temperature range (K), max.	594.02

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermochemistry of Li, Na, K, Rb and Cs alkylated phenoxides: https://www.doi.org/10.1016/j.tca.2005.02.027

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=C128392&Units=SI

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

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

hfust: Enthalpy of fusion at a given temperature

hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume