Phenol, 2,5-bis(1,1-dimethylethyl)-

Other names:	Phenol, 2,5-di-tert-butyl-
	2,5-Di-tert-butylphenol
	2,5-bis(1,1-Dimethylethyl)phenol
Inchi:	InChI=1S/C14H22O/c1-13(2,3)10-7-8-11(12(15)9-10)14(4,5)6/h7-9,15H,1-6H3
InchiKey:	KDBZVULQVCUNNA-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)c1ccc(C(C)(C)C)c(O)c1
Mol. weight [g/mol]:	206.32
CAS:	5875-45-6

Physical Properties

Property code	Value	Unit	Source
chs	-8276.00	kJ/mol	NIST Webbook
gf	20.84	kJ/mol	Joback Method
hf	-260.00	kJ/mol	NIST Webbook
hfs	-380.00	kJ/mol	NIST Webbook
hfus	16.62	kJ/mol	Joback Method
hsub	120.00	kJ/mol	NIST Webbook
hsub	116.70	kJ/mol	NIST Webbook
hvap	60.12	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.987		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1514.00		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	588.49	J/mol×K	817.41	Joback Method
cpg	575.03	J/mol×K	779.03	Joback Method
cpg	560.71	J/mol×K	740.66	Joback Method
cpg	545.39	J/mol×K	702.29	Joback Method
cpg	528.92	J/mol×K	663.91	Joback Method
cpg	601.25	J/mol×K	855.78	Joback Method
dvisc	0.0000185	Pa×s	625.54	Joback Method
dvisc	0.0000295	Pa×s	588.46	Joback Method
dvisc	0.0000499	Pa×s	551.37	Joback Method
dvisc	0.0000911	Pa×s	514.29	Joback Method
dvisc	0.0001828	Pa×s	477.21	Joback Method
dvisc	0.0004121	Pa×s	440.12	Joback Method
dvisc	0.0010791	Pa×s	403.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5875456&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

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
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

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume