Phenol, 2-chloro-4-(1,1,3,3-tetramethylbutyl)-

Inchi: InChI=1S/C14H21ClO/c1-13(2,3)9-14(4,5)10-6-7-12(16)11(15)8-10/h6-8,16H,9H2,1-5H3
InchiKey: CLYCAZNGUGDEBH-UHFFFAOYSA-N
Formula: C14H21ClO
SMILES: CC(C)(C)CC(C)(C)c1ccc(O)c(Cl)c1
Mol. weight [g/mol]: 240.77
CAS: 17199-24-5

Physical Properties

Property code	Value	Unit	Source
gf	8.91	kJ/mol	Joback Method
hf	-317.78	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.759		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	662.97	K	Joback Method
tc	896.28	K	Joback Method
tf	432.96	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.54	J/mol×K	662.97	Joback Method
cpg	611.16	J/mol×K	857.40	Joback Method
cpg	598.58	J/mol×K	818.51	Joback Method
cpg	585.28	J/mol×K	779.63	Joback Method
cpg	571.12	J/mol×K	740.74	Joback Method
cpg	555.92	J/mol×K	701.86	Joback Method
cpg	623.17	J/mol×K	896.28	Joback Method

dvisc	0.0000138	Pa×s	662.97	Joback Method
dvisc	0.0000214	Pa×s	624.63	Joback Method
dvisc	0.0000354	Pa×s	586.30	Joback Method
dvisc	0.0000625	Pa×s	547.97	Joback Method
dvisc	0.0001204	Pa×s	509.63	Joback Method
dvisc	0.0002581	Pa×s	471.29	Joback Method
dvisc	0.0006330	Pa×s	432.96	Joback Method

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=C17199245&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume