2,4-Ditert-butyl-6-chlorophenol

Other names:	Phenol, 4,6-di-tert-butyl-2-chloro-
Inchi:	InChI=1S/C14H21ClO/c1-13(2,3)9-7-10(14(4,5)6)12(16)11(15)8-9/h7-8,16H,1-6H3
InchiKey:	CWSNVVXDGQVVDZ-UHFFFAOYSA-N
Formula:	C14H21ClO
SMILES:	CC(C)(C)c1cc(Cl)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	240.77
CAS:	4166-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-0.72	kJ/mol	Joback Method
hf	-329.25	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	65.16	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.641		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
tb	667.95	K	Joback Method
tc	902.14	K	Joback Method
tf	445.48	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.77	J/mol×K	667.95	Joback Method
cpg	554.94	J/mol×K	706.98	Joback Method
cpg	569.99	J/mol×K	746.01	Joback Method
cpg	584.06	J/mol×K	785.04	Joback Method
cpg	597.29	J/mol×K	824.07	Joback Method
cpg	609.84	J/mol×K	863.11	Joback Method
cpg	621.86	J/mol×K	902.14	Joback Method
dvisc	0.0004546	Pa×s	445.48	Joback Method

dvisc	0.0002012	Pa×s	482.56	Joback Method
dvisc	0.0001001	Pa×s	519.64	Joback Method
dvisc	0.0000546	Pa×s	556.72	Joback Method
dvisc	0.0000321	Pa×s	593.79	Joback Method
dvisc	0.0000201	Pa×s	630.87	Joback Method
dvisc	0.0000133	Pa×s	667.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4166863&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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