

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.77	J/mol×K	667.95	Joback Method
cpg	609.84	J/mol×K	863.11	Joback Method
cpg	597.29	J/mol×K	824.07	Joback Method
cpg	584.06	J/mol×K	785.04	Joback Method
cpg	569.99	J/mol×K	746.01	Joback Method
cpg	554.94	J/mol×K	706.98	Joback Method
cpg	621.86	J/mol×K	902.14	Joback Method
dvisc	0.0000133	Paxs	667.95	Joback Method

dvisc	0.0000201	Paxs	630.87	Joback Method
dvisc	0.0000321	Paxs	593.79	Joback Method
dvisc	0.0000546	Paxs	556.72	Joback Method
dvisc	0.0001001	Paxs	519.64	Joback Method
dvisc	0.0002012	Paxs	482.56	Joback Method
dvisc	0.0004546	Paxs	445.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4166863&Units=SI

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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