

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

Other names:	Phenol, 2-tert-butyl-6-chloro- 2-Tert-butyl-6-chlorophenol
Inchi:	InChI=1S/C10H13ClO/c1-10(2,3)7-5-4-6-8(11)9(7)12/h4-6,12H,1-3H3
InchiKey:	UBHJDCKSYYGMRI-UHFFFAOYSA-N
Formula:	C10H13ClO
SMILES:	CC(C)(C)c1cccc(Cl)c1O
Mol. weight [g/mol]:	184.66
CAS:	4237-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-27.61	kJ/mol	Joback Method
hf	-226.47	kJ/mol	Joback Method
hfus	17.87	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.343		Crippen Method
mvol	146.110	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	574.68	K	Joback Method
tc	812.94	K	Joback Method
tf	385.46	K	Joback Method
vc	0.491	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.45	J/molxK	574.68	Joback Method
cpg	353.77	J/molxK	614.39	Joback Method
cpg	366.02	J/molxK	654.10	Joback Method
cpg	377.32	J/molxK	693.81	Joback Method
cpg	387.80	J/molxK	733.52	Joback Method
cpg	397.57	J/molxK	773.23	Joback Method
cpg	406.76	J/molxK	812.94	Joback Method

dvisc	0.0014414	Paxs	385.46	Joback Method
dvisc	0.0006374	Paxs	417.00	Joback Method
dvisc	0.0003161	Paxs	448.53	Joback Method
dvisc	0.0001719	Paxs	480.07	Joback Method
dvisc	0.0001008	Paxs	511.61	Joback Method
dvisc	0.0000629	Paxs	543.14	Joback Method
dvisc	0.0000413	Paxs	574.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4237370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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