Phenol, 2,6-dichloro-4-(1-methylpropyl)-

Other names: 4-Sec-butyl-2,6-dichlorophenol
Inchi: InChI=1S/C10H12Cl2O/c1-3-6(2)7-4-8(11)10(13)9(12)5-7/h4-6,13H,3H2,1-2H3
InchiKey: DZKJAGRVOGNQGW-UHFFFAOYSA-N
Formula: C10H12Cl2O
SMILES: CCC(C)c1cc(Cl)c(O)c(Cl)c1
Mol. weight [g/mol]: 219.11
CAS: 34593-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-54.45	kJ/mol	Joback Method
hf	-250.21	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	4.213		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	619.88	K	Joback Method
tc	853.16	K	Joback Method
tf	410.48	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.17	J/mol×K	619.88	Joback Method
cpg	371.82	J/mol×K	658.76	Joback Method
cpg	382.70	J/mol×K	697.64	Joback Method
cpg	392.88	J/mol×K	736.52	Joback Method
cpg	402.46	J/mol×K	775.40	Joback Method
cpg	411.52	J/mol×K	814.28	Joback Method
cpg	420.13	J/mol×K	853.16	Joback Method
dvisc	0.0008848	Pa×s	410.48	Joback Method

dvisc	0.0004064	Pa×s	445.38	Joback Method
dvisc	0.0002090	Pa×s	480.28	Joback Method
dvisc	0.0001176	Pa×s	515.18	Joback Method
dvisc	0.0000712	Pa×s	550.08	Joback Method
dvisc	0.0000457	Pa×s	584.98	Joback Method
dvisc	0.0000309	Pa×s	619.88	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=C34593743&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume