2,6-Diallyl-4-chlorophenol

Inchi: InChI=1S/C12H13ClO/c1-3-5-9-7-11(13)8-10(6-4-2)12(9)14/h3-4,7-8,14H,1-2,5-6H2
InchiKey: RANSQHWYECVCMB-UHFFFAOYSA-N
Formula: C12H13ClO
SMILES: C=CCc1cc(Cl)cc(CC=C)c1O
Mol. weight [g/mol]: 208.68
CAS: 73267-76-2

Physical Properties

Property code	Value	Unit	Source
gf	152.44	kJ/mol	Joback Method
hf	-19.61	kJ/mol	Joback Method
hfus	27.52	kJ/mol	Joback Method
hvap	61.97	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.503		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	622.01	K	Joback Method
tc	847.72	K	Joback Method
tf	414.58	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.58	J/mol×K	622.01	Joback Method
cpg	443.42	J/mol×K	810.10	Joback Method
cpg	433.71	J/mol×K	772.48	Joback Method
cpg	423.46	J/mol×K	734.86	Joback Method
cpg	412.58	J/mol×K	697.25	Joback Method
cpg	400.98	J/mol×K	659.63	Joback Method
cpg	452.68	J/mol×K	847.72	Joback Method
dvisc	0.0000306	Pa×s	622.01	Joback Method
dvisc	0.0000443	Pa×s	587.44	Joback Method

dvisc	0.0000673	Pa×s	552.87	Joback Method
dvisc	0.0001081	Pa×s	518.30	Joback Method
dvisc	0.0001858	Pa×s	483.72	Joback Method
dvisc	0.0003469	Pa×s	449.15	Joback Method
dvisc	0.0007190	Pa×s	414.58	Joback Method

Sources

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=C73267762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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