

2-Allyl-3,6-dichlorophenol

Inchi:	InChI=1S/C9H8Cl2O/c1-2-3-6-7(10)4-5-8(11)9(6)12/h2,4-5,12H,1,3H2
InchiKey:	RDUKRQJHXBCYIY-UHFFFAOYSA-N
Formula:	C9H8Cl2O
SMILES:	C=CCc1c(Cl)ccc(Cl)c1O
Mol. weight [g/mol]:	203.06
CAS:	116632-92-9

Physical Properties

Property code	Value	Unit	Source
gf	27.41	kJ/mol	Joback Method
hf	-98.86	kJ/mol	Joback Method
hfus	25.23	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.428		Crippen Method
mcvol	139.960	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	594.12	K	Joback Method
tc	832.22	K	Joback Method
tf	412.45	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.25	J/molxK	594.12	Joback Method
cpg	335.05	J/molxK	792.54	Joback Method
cpg	327.75	J/molxK	752.86	Joback Method
cpg	320.02	J/molxK	713.17	Joback Method
cpg	311.75	J/molxK	673.49	Joback Method
cpg	302.85	J/molxK	633.80	Joback Method
cpg	341.99	J/molxK	832.22	Joback Method
dvisc	0.0000437	Paxs	594.12	Joback Method
dvisc	0.0000621	Paxs	563.84	Joback Method

dvisc	0.0000918	Paxs	533.56	Joback Method
dvisc	0.0001421	Paxs	503.29	Joback Method
dvisc	0.0002327	Paxs	473.01	Joback Method
dvisc	0.0004078	Paxs	442.73	Joback Method
dvisc	0.0007758	Paxs	412.45	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=C116632929&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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