

Allyl-2,3,6-trichlorophenyl ether

Inchi:	InChI=1S/C9H7Cl3O/c1-2-5-13-9-7(11)4-3-6(10)8(9)12/h2-4H,1,5H2
InchiKey:	GYMHSNQIWMTIOZ-UHFFFAOYSA-N
Formula:	C9H7Cl3O
SMILES:	C=CCOc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	237.51
CAS:	116435-14-4

Physical Properties

Property code	Value	Unit	Source
gf	55.47	kJ/mol	Joback Method
hf	-80.98	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.212		Crippen Method
mcvol	152.200	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	578.33	K	Joback Method
tc	807.72	K	Joback Method
tf	365.40	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.43	J/molxK	578.33	Joback Method
cpg	336.60	J/molxK	769.49	Joback Method
cpg	329.10	J/molxK	731.26	Joback Method
cpg	321.04	J/molxK	693.03	Joback Method
cpg	312.42	J/molxK	654.79	Joback Method
cpg	303.22	J/molxK	616.56	Joback Method
cpg	343.56	J/molxK	807.72	Joback Method
dvisc	0.0002005	Paxs	578.33	Joback Method
dvisc	0.0002405	Paxs	542.84	Joback Method

dvisc	0.0002959	Paxs	507.35	Joback Method
dvisc	0.0003755	Paxs	471.87	Joback Method
dvisc	0.0004955	Paxs	436.38	Joback Method
dvisc	0.0006867	Paxs	400.89	Joback Method
dvisc	0.0010139	Paxs	365.40	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=C116435144&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

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