

1,2,4-Trichloro-5-isopropoxybenzene

Inchi:	InChI=1S/C9H9Cl3O/c1-5(2)13-9-4-7(11)6(10)3-8(9)12/h3-5H,1-2H3
InchiKey:	KRWAFSMISJEYKC-UHFFFAOYSA-N
Formula:	C9H9Cl3O
SMILES:	CC(C)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	239.53
CAS:	6851-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.81	kJ/mol	Joback Method
hf	-211.69	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	55.07	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.434		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	581.21	K	Joback Method
tc	810.67	K	Joback Method
tf	352.16	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.71	J/mol×K	581.21	Joback Method
cpg	324.62	J/mol×K	619.45	Joback Method
cpg	334.89	J/mol×K	657.70	Joback Method
cpg	344.54	J/mol×K	695.94	Joback Method
cpg	353.58	J/mol×K	734.18	Joback Method
cpg	362.00	J/mol×K	772.43	Joback Method
cpg	369.83	J/mol×K	810.67	Joback Method
dvisc	0.0012326	Pa×s	352.16	Joback Method
dvisc	0.0007663	Pa×s	390.34	Joback Method

dvisc	0.0005185	Pa×s	428.51	Joback Method
dvisc	0.0003740	Pa×s	466.69	Joback Method
dvisc	0.0002834	Pa×s	504.86	Joback Method
dvisc	0.0002233	Pa×s	543.04	Joback Method
dvisc	0.0001816	Pa×s	581.21	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=C6851463&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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