1,2,4-Trichloro-5-(2-chloroethoxy)benzene

Inchi: InChI=1S/C8H6Cl4O/c9-1-2-13-8-4-6(11)5(10)3-7(8)12/h3-4H,1-2H2
InchiKey: QRAXLUVIRXAFDT-UHFFFAOYSA-N
Formula: C8H6Cl4O
SMILES: ClCCOc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 259.94
CAS: 101654-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-52.72	kJ/mol	Joback Method
hf	-201.51	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	57.61	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.264		Crippen Method
mcvol	154.650	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	596.20	K	Joback Method
tc	828.89	K	Joback Method
tf	385.81	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.13	J/mol×K	596.20	Joback Method
cpg	328.84	J/mol×K	790.11	Joback Method
cpg	322.16	J/mol×K	751.33	Joback Method
cpg	314.96	J/mol×K	712.55	Joback Method
cpg	307.23	J/mol×K	673.76	Joback Method
cpg	298.95	J/mol×K	634.98	Joback Method
cpg	334.98	J/mol×K	828.89	Joback Method
dvisc	0.0002033	Pa×s	596.20	Joback Method
dvisc	0.0002442	Pa×s	561.13	Joback Method

dvisc	0.0003006	Pa×s	526.07	Joback Method
dvisc	0.0003813	Pa×s	491.00	Joback Method
dvisc	0.0005016	Pa×s	455.94	Joback Method
dvisc	0.0006907	Pa×s	420.88	Joback Method
dvisc	0.0010081	Pa×s	385.81	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C101654233&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