Benzene, 1,2-bis-(chloromethyl)-4-chloro

Inchi: InChI=1S/C8H7Cl3/c9-4-6-1-2-8(11)3-7(6)5-10/h1-3H,4-5H2
InchiKey: SBXAWQQSJQEERL-UHFFFAOYSA-N
Formula: C8H7Cl3
SMILES: ClCc1ccc(Cl)cc1CCl
Mol. weight [g/mol]: 209.50

Physical Properties

Property code	Value	Unit	Source
gf	73.84	kJ/mol	Joback Method
hf	-42.08	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	50.16	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.818		Crippen Method
mcvol	136.540	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
tb	531.37	K	Joback Method
tc	762.04	K	Joback Method
tf	321.14	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.14	J/mol×K	531.37	Joback Method
cpg	259.06	J/mol×K	569.82	Joback Method
cpg	268.33	J/mol×K	608.26	Joback Method
cpg	276.97	J/mol×K	646.71	Joback Method
cpg	285.01	J/mol×K	685.15	Joback Method
cpg	292.49	J/mol×K	723.60	Joback Method
cpg	299.43	J/mol×K	762.04	Joback Method
dvisc	0.0017127	Pa×s	321.14	Joback Method

dvisc	0.0010789	Pa×s	356.18	Joback Method
dvisc	0.0007383	Pa×s	391.22	Joback Method
dvisc	0.0005378	Pa×s	426.25	Joback Method
dvisc	0.0004110	Pa×s	461.29	Joback Method
dvisc	0.0003263	Pa×s	496.33	Joback Method
dvisc	0.0002670	Pa×s	531.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131630&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume