Benzene, 4-chloro-1,3-bis-(chloromethyl)-5-methyl

Inchi: InChI=1S/C9H9Cl3/c1-6-2-7(4-10)3-8(5-11)9(6)12/h2-3H,4-5H2,1H3
InchiKey: XMAVRXJRPJQEAB-UHFFFAOYSA-N
Formula: C9H9Cl3
SMILES: Cc1cc(CCl)cc(CCl)c1Cl
Mol. weight [g/mol]: 223.53

Physical Properties

Property code	Value	Unit	Source
gf	72.63	kJ/mol	Joback Method
hf	-74.19	kJ/mol	Joback Method
hfus	24.53	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.126		Crippen Method
mcvol	150.630	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1566.00		NIST Webbook
tb	559.23	K	Joback Method
tc	786.70	K	Joback Method
tf	344.93	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.33	J/mol×K	559.23	Joback Method
cpg	338.72	J/mol×K	748.79	Joback Method
cpg	330.44	J/mol×K	710.88	Joback Method
cpg	321.58	J/mol×K	672.96	Joback Method
cpg	312.13	J/mol×K	635.05	Joback Method
cpg	302.05	J/mol×K	597.14	Joback Method
cpg	346.45	J/mol×K	786.70	Joback Method
dvisc	0.0002404	Pa×s	559.23	Joback Method
dvisc	0.0002905	Pa×s	523.51	Joback Method

dvisc	0.0003609	Pa×s	487.80	Joback Method
dvisc	0.0004640	Pa×s	452.08	Joback Method
dvisc	0.0006229	Pa×s	416.36	Joback Method
dvisc	0.0008836	Pa×s	380.65	Joback Method
dvisc	0.0013475	Pa×s	344.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132153&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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