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

Inchi: InChI=1S/C8H8Cl2/c1-6-2-3-8(10)7(4-6)5-9/h2-4H,5H2,1H3
InchiKey: PYEZGJNZDIRIIM-UHFFFAOYSA-N
Formula: C8H8Cl2
SMILES: Cc1ccc(Cl)c(CCl)c1
Mol. weight [g/mol]: 175.06

Physical Properties

Property code	Value	Unit	Source
gf	85.77	kJ/mol	Joback Method
hf	-26.34	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.387		Crippen Method
mcvol	124.300	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1238.00		NIST Webbook
tb	493.94	K	Joback Method
tc	719.52	K	Joback Method
tf	291.22	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.48	J/mol×K	493.94	Joback Method
cpg	237.10	J/mol×K	531.54	Joback Method
cpg	247.09	J/mol×K	569.13	Joback Method
cpg	256.47	J/mol×K	606.73	Joback Method
cpg	265.25	J/mol×K	644.33	Joback Method
cpg	273.48	J/mol×K	681.92	Joback Method
cpg	281.16	J/mol×K	719.52	Joback Method
dvisc	0.0017277	Pa×s	291.22	Joback Method
dvisc	0.0010719	Pa×s	325.01	Joback Method

dvisc	0.0007276	Pa×s	358.79	Joback Method
dvisc	0.0005279	Pa×s	392.58	Joback Method
dvisc	0.0004030	Pa×s	426.37	Joback Method
dvisc	0.0003201	Pa×s	460.15	Joback Method
dvisc	0.0002624	Pa×s	493.94	Joback Method

Sources

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=R132188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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