Benzene, 4-chloro-5-(chloromethyl)-1,3-dimethyl

Inchi: InChI=1S/C9H10Cl2/c1-6-3-7(2)9(11)8(4-6)5-10/h3-4H,5H2,1-2H3
InchiKey: GYCLOBCJCWLHFD-UHFFFAOYSA-N
Formula: C9H10Cl2
SMILES: Cc1cc(C)c(Cl)c(CCl)c1
Mol. weight [g/mol]: 189.08

Physical Properties

Property code	Value	Unit	Source
gf	84.56	kJ/mol	Joback Method
hf	-58.45	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	48.66	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.696		Crippen Method
mcvol	138.390	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
tb	521.80	K	Joback Method
tc	744.72	K	Joback Method
tf	315.01	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.93	J/mol×K	521.80	Joback Method
cpg	279.37	J/mol×K	558.95	Joback Method
cpg	290.18	J/mol×K	596.11	Joback Method
cpg	300.38	J/mol×K	633.26	Joback Method
cpg	309.99	J/mol×K	670.42	Joback Method
cpg	319.02	J/mol×K	707.57	Joback Method
cpg	327.51	J/mol×K	744.72	Joback Method
dvisc	0.0013611	Pa×s	315.01	Joback Method

dvisc	0.0008835	Pa×s	349.47	Joback Method
dvisc	0.0006198	Pa×s	383.94	Joback Method
dvisc	0.0004610	Pa×s	418.40	Joback Method
dvisc	0.0003586	Pa×s	452.87	Joback Method
dvisc	0.0002891	Pa×s	487.33	Joback Method
dvisc	0.0002398	Pa×s	521.80	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=R132202&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
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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