

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
mvol	138.390	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1348.00		NIST Webbook
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tb	521.80	K	Joback Method
tc	744.72	K	Joback Method
tf	315.01	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0008835	Paxs	349.47	Joback Method
dvisc	0.0006198	Paxs	383.94	Joback Method
dvisc	0.0004610	Paxs	418.40	Joback Method
dvisc	0.0003586	Paxs	452.87	Joback Method
dvisc	0.0002891	Paxs	487.33	Joback Method
dvisc	0.0002398	Paxs	521.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R132202&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
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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