

Benzene, 1,3-dichloro-5-(chloromethyl)-

Inchi:	InChI=1S/C7H5Cl3/c8-4-5-1-6(9)3-7(10)2-5/h1-3H,4H2
InchiKey:	ZFLRKAMKGYNFPH-UHFFFAOYSA-N
Formula:	C7H5Cl3
SMILES:	ClCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	195.47
CAS:	3290-06-0

Physical Properties

Property code	Value	Unit	Source
gf	65.42	kJ/mol	Joback Method
hf	-21.44	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	47.93	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.732		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	508.49	K	Joback Method
tc	743.54	K	Joback Method
tf	309.87	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.02	J/molxK	508.49	Joback Method
cpg	245.65	J/molxK	704.37	Joback Method
cpg	239.19	J/molxK	665.19	Joback Method
cpg	232.23	J/molxK	626.02	Joback Method
cpg	224.73	J/molxK	586.84	Joback Method
cpg	216.67	J/molxK	547.67	Joback Method
cpg	251.62	J/molxK	743.54	Joback Method
dvisc	0.0002870	Paxs	508.49	Joback Method
dvisc	0.0003484	Paxs	475.39	Joback Method

dvisc	0.0004353	Paxs	442.28	Joback Method
dvisc	0.0005638	Paxs	409.18	Joback Method
dvisc	0.0007643	Paxs	376.08	Joback Method
dvisc	0.0010988	Paxs	342.97	Joback Method
dvisc	0.0017070	Paxs	309.87	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=C3290060&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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