

Benzene, 2-chloro-5-(chloromethyl)-1-methyl

Inchi:	InChI=1S/C8H8Cl2/c1-6-4-7(5-9)2-3-8(6)10/h2-4H,5H2,1H3
InchiKey:	BNINSXCMJBCDPZ-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	Cc1cc(CCl)ccc1Cl
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	1230.00		NIST Webbook
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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/molxK	493.94	Joback Method
cpg	273.48	J/molxK	681.92	Joback Method
cpg	265.25	J/molxK	644.33	Joback Method
cpg	256.47	J/molxK	606.73	Joback Method
cpg	247.09	J/molxK	569.13	Joback Method
cpg	237.10	J/molxK	531.54	Joback Method
cpg	281.16	J/molxK	719.52	Joback Method
dvisc	0.0002624	Paxs	493.94	Joback Method

dvisc	0.0003201	Paxs	460.15	Joback Method
dvisc	0.0004030	Paxs	426.37	Joback Method
dvisc	0.0005279	Paxs	392.58	Joback Method
dvisc	0.0007276	Paxs	358.79	Joback Method
dvisc	0.0010719	Paxs	325.01	Joback Method
dvisc	0.0017277	Paxs	291.22	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=R132039&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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