

Benzene, 1-(chloromethyl)-2,3-dimethyl

Inchi:	InChI=1S/C9H11Cl/c1-7-4-3-5-9(6-10)8(7)2/h3-5H,6H2,1-2H3
InchiKey:	CHMJJIHXWABUHA-UHFFFAOYSA-N
Formula:	C9H11Cl
SMILES:	Cc1cccc(CCl)c1C
Mol. weight [g/mol]:	154.64

Physical Properties

Property code	Value	Unit	Source
gf	106.12	kJ/mol	Joback Method
hf	-31.24	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	43.61	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.042		Crippen Method
mvol	126.150	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
tb	479.39	K	Joback Method
tc	695.70	K	Joback Method
tf	272.57	K	Joback Method
vc	0.480	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.19	J/molxK	479.39	Joback Method
cpg	299.10	J/molxK	659.65	Joback Method
cpg	289.18	J/molxK	623.60	Joback Method
cpg	278.64	J/molxK	587.55	Joback Method
cpg	267.48	J/molxK	551.49	Joback Method
cpg	255.67	J/molxK	515.44	Joback Method
cpg	308.45	J/molxK	695.70	Joback Method
dvisc	0.0002356	Paxs	479.39	Joback Method

dvisc	0.0002888	Paxs	444.92	Joback Method
dvisc	0.0003664	Paxs	410.45	Joback Method
dvisc	0.0004855	Paxs	375.98	Joback Method
dvisc	0.0006809	Paxs	341.51	Joback Method
dvisc	0.0010303	Paxs	307.04	Joback Method
dvisc	0.0017313	Paxs	272.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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