Benzene, 1-(1-chloroethyl)-4-methyl

Inchi: InChI=1S/C9H11Cl/c1-7-3-5-9(6-4-7)8(2)10/h3-6,8H,1-2H3
InchiKey: WQLQKKZHEUQVBU-UHFFFAOYSA-N
Formula: C9H11Cl
SMILES: Cc1ccc(C(C)Cl)cc1
Mol. weight [g/mol]: 154.64

Physical Properties

Property code	Value	Unit	Source
gf	113.31	kJ/mol	Joback Method
hf	-25.05	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.295		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1149.00		NIST Webbook
tb	473.97	K	Joback Method
tc	694.11	K	Joback Method
tf	245.05	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.09	J/mol×K	473.97	Joback Method
cpg	256.40	J/mol×K	510.66	Joback Method
cpg	268.93	J/mol×K	547.35	Joback Method
cpg	280.70	J/mol×K	584.04	Joback Method
cpg	291.74	J/mol×K	620.73	Joback Method
cpg	302.10	J/mol×K	657.42	Joback Method
cpg	311.78	J/mol×K	694.11	Joback Method
dvisc	0.0033321	Pa×s	245.05	Joback Method
dvisc	0.0015870	Pa×s	283.20	Joback Method

dvisc	0.0009014	Pa×s	321.36	Joback Method
dvisc	0.0005773	Pa×s	359.51	Joback Method
dvisc	0.0004028	Pa×s	397.66	Joback Method
dvisc	0.0002993	Pa×s	435.82	Joback Method
dvisc	0.0002333	Pa×s	473.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129647&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