(1-Chloro-1-methylethyl)benzene

Other names: Alpha,alpha-dimethylbenzyl chloride
Benzene, (1-chloro-1-methylethyl)-
Inchi: InChI=1S/C9H11Cl/c1-9(2,10)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey: KPJKMUJJFXZGAX-UHFFFAOYSA-N
Formula: C9H11Cl
SMILES: CC(C)(Cl)c1ccccc1
Mol. weight [g/mol]: 154.64
CAS: 934-53-2

Physical Properties

Property code	Value	Unit	Source
gf	128.22	kJ/mol	Joback Method
hf	-17.05	kJ/mol	Joback Method
hfl	-76.00 ± 3.00	kJ/mol	NIST Webbook
hfus	9.89	kJ/mol	Joback Method
hvap	54.70	kJ/mol	NIST Webbook
log10ws	-3.01		Crippen Method
logp	3.161		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1109.00		NIST Webbook
tb	466.20	K	Joback Method
tc	694.75	K	Joback Method
tf	249.95	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.35	J/mol×K	466.20	Joback Method

cpg	260.08	J/mol×K	504.29	Joback Method
cpg	273.70	J/mol×K	542.38	Joback Method
cpg	286.27	J/mol×K	580.47	Joback Method
cpg	297.86	J/mol×K	618.57	Joback Method
cpg	308.54	J/mol×K	656.66	Joback Method
cpg	318.38	J/mol×K	694.75	Joback Method
dvisc	0.0050419	Pa×s	249.95	Joback Method
dvisc	0.0022467	Pa×s	285.99	Joback Method
dvisc	0.0011997	Pa×s	322.03	Joback Method
dvisc	0.0007269	Pa×s	358.08	Joback Method
dvisc	0.0004827	Pa×s	394.12	Joback Method
dvisc	0.0003433	Pa×s	430.16	Joback Method
dvisc	0.0002573	Pa×s	466.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38272e+01
Coeff. B	-3.79701e+03
Coeff. C	-7.51370e+01
Temperature range (K), min.	355.57
Temperature range (K), max.	521.02

Sources

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=C934532&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume