Benzene, 1-bromo-2-(chloromethyl)-

Inchi: InChI=1S/C7H6BrCl/c8-7-4-2-1-3-6(7)5-9/h1-4H,5H2
InchiKey: DDVSFIUKWUTKES-UHFFFAOYSA-N
Formula: C7H6BrCl
SMILES: ClCc1ccccc1Br
Mol. weight [g/mol]: 205.48
CAS: 578-51-8

Physical Properties

Property code	Value	Unit	Source
gf	113.23	kJ/mol	Joback Method
hf	47.84	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	44.93	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.188		Crippen Method
mcvol	115.470	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	494.81	K	Joback Method
tc	734.55	K	Joback Method
tf	297.31	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.64	J/mol×K	494.81	Joback Method
cpg	237.24	J/mol×K	694.60	Joback Method
cpg	230.19	J/mol×K	654.64	Joback Method
cpg	222.55	J/mol×K	614.68	Joback Method
cpg	214.28	J/mol×K	574.72	Joback Method
cpg	205.32	J/mol×K	534.77	Joback Method
cpg	243.74	J/mol×K	734.55	Joback Method

dvisc	0.0003139	Pa×s	494.81	Joback Method
dvisc	0.0003844	Pa×s	461.89	Joback Method
dvisc	0.0004857	Pa×s	428.98	Joback Method
dvisc	0.0006381	Pa×s	396.06	Joback Method
dvisc	0.0008806	Pa×s	363.14	Joback Method
dvisc	0.0012960	Pa×s	330.23	Joback Method
dvisc	0.0020778	Pa×s	297.31	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C578518&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
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