

Benzene, 1-bromo-4-(chloromethyl)-

Other names:	1-bromo-4-(chloromethyl)benzene
Inchi:	InChI=1S/C7H6BrCl/c8-7-3-1-6(5-9)2-4-7/h1-4H,5H2
InchiKey:	BSIIGUGKOPPTPZ-UHFFFAOYSA-N
Formula:	C7H6BrCl
SMILES:	ClCc1ccc(Br)cc1
Mol. weight [g/mol]:	205.48
CAS:	589-17-3

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
tb	511.00	K	NIST Webbook
tc	734.55	K	Joback Method
tf	323.00	K	NIST Webbook
tf	314.90 ± 4.00	K	NIST Webbook
vc	0.430	m ³ /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	Paxs	494.81	Joback Method
dvisc	0.0003844	Paxs	461.89	Joback Method
dvisc	0.0004857	Paxs	428.98	Joback Method
dvisc	0.0006381	Paxs	396.06	Joback Method
dvisc	0.0008806	Paxs	363.14	Joback Method
dvisc	0.0012960	Paxs	330.23	Joback Method
dvisc	0.0020778	Paxs	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=C589173&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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