Benzene, 1-(2-bromoethyl)-3-chloro-

Other names: 1-Bromo-2-(3-chlorophenyl)ethane
Inchi: InChI=1S/C8H8BrCl/c9-5-4-7-2-1-3-8(10)6-7/h1-3,6H,4-5H2
InchiKey: LKPWGXCMVLJRIK-UHFFFAOYSA-N
Formula: C8H8BrCl
SMILES: Clc1cccc(CCBr)c1
Mol. weight [g/mol]: 219.51
CAS: 16799-05-6

Physical Properties

Property code	Value	Unit	Source
gf	121.65	kJ/mol	Joback Method
hf	27.20	kJ/mol	Joback Method
hfus	19.61	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-3.39		Crippen Method
logp	3.277		Crippen Method
mcvol	129.560	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	517.69	K	Joback Method
tc	752.93	K	Joback Method
tf	308.58	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.61	J/mol×K	517.69	Joback Method
cpg	283.93	J/mol×K	713.72	Joback Method
cpg	275.84	J/mol×K	674.52	Joback Method
cpg	267.11	J/mol×K	635.31	Joback Method
cpg	257.70	J/mol×K	596.10	Joback Method
cpg	247.55	J/mol×K	556.90	Joback Method
cpg	291.42	J/mol×K	752.93	Joback Method

dvisc	0.0002907	Pa×s	517.69	Joback Method
dvisc	0.0003584	Pa×s	482.84	Joback Method
dvisc	0.0004565	Pa×s	447.99	Joback Method
dvisc	0.0006058	Pa×s	413.14	Joback Method
dvisc	0.0008468	Pa×s	378.28	Joback Method
dvisc	0.0012669	Pa×s	343.43	Joback Method
dvisc	0.0020762	Pa×s	308.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16799056&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ie:	Ionization energy
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