Benzene, 1-(2-bromoethyl)-4-chloro-

Other names:	p-Chloro-«beta»-phenethyl bromide
	p-Chlorophenethyl bromide
	1-(2-Bromoethyl)-4-chlorobenzene
	2-(p-Chlorophenyl)ethyl bromide
	4-Chlorophenethyl bromide
	1-Bromo-2-(4-chlorophenyl)ethane
Inchi:	InChI=1S/C8H8BrCl/c9-6-5-7-1-3-8(10)4-2-7/h1-4H,5-6H2
InchiKey:	YAFMYKFAUNCQPU-UHFFFAOYSA-N
Formula:	C8H8BrCl
SMILES:	Clc1ccc(CCBr)cc1
Mol. weight [g/mol]:	219.51
CAS:	6529-53-9

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	8.80	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	247.55	J/mol×K	556.90	Joback Method

cpg	257.70	J/mol×K	596.10	Joback Method
cpg	267.11	J/mol×K	635.31	Joback Method
cpg	275.84	J/mol×K	674.52	Joback Method
cpg	283.93	J/mol×K	713.72	Joback Method
cpg	291.42	J/mol×K	752.93	Joback Method
dvisc	0.0020762	Pa×s	308.58	Joback Method
dvisc	0.0012669	Pa×s	343.43	Joback Method
dvisc	0.0008468	Pa×s	378.28	Joback Method
dvisc	0.0006058	Pa×s	413.14	Joback Method
dvisc	0.0004565	Pa×s	447.99	Joback Method
dvisc	0.0003584	Pa×s	482.84	Joback Method
dvisc	0.0002907	Pa×s	517.69	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6529539&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