

Aniline, 2-bromo-6-chloro

Inchi:	InChI=1S/C6H5BrClN/c7-4-2-1-3-5(8)6(4)9/h1-3H,9H2
InchiKey:	BIMSFWCFKDVSNO-UHFFFAOYSA-N
Formula:	C6H5BrClN
SMILES:	Nc1c(Cl)cccc1Br
Mol. weight [g/mol]:	206.47

Physical Properties

Property code	Value	Unit	Source
gf	161.63	kJ/mol	Joback Method
hf	90.80	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.685		Crippen Method
mcvol	111.360	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
rinpol	1284.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1284.00		NIST Webbook
tb	549.44	K	Joback Method
tc	805.41	K	Joback Method
tf	381.82	K	Joback Method
vc	0.404	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.79	J/molxK	549.44	Joback Method
cpg	206.83	J/molxK	592.10	Joback Method
cpg	214.23	J/molxK	634.76	Joback Method
cpg	221.04	J/molxK	677.42	Joback Method
cpg	227.30	J/molxK	720.08	Joback Method
cpg	233.04	J/molxK	762.74	Joback Method
cpg	238.31	J/molxK	805.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R621826&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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