

5-Bromovaleronitrile

Other names:	Pentanenitrile, 5-bromo- Valeronitrile, delta-bromo- 5-bromopentanenitrile
Inchi:	InChI=1S/C5H8BrN/c6-4-2-1-3-5-7/h1-4H2
InchiKey:	NWWWGAKVHCSAEU-UHFFFAOYSA-N
Formula:	C5H8BrN
SMILES:	N#CCCCCB
Mol. weight [g/mol]:	162.03
CAS:	5414-21-1

Physical Properties

Property code	Value	Unit	Source
gf	138.72	kJ/mol	Joback Method
hf	44.68	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	43.64	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.075		Crippen Method
mcvol	100.190	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	482.04	K	Joback Method
tc	690.14	K	Joback Method
tf	270.90	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.78	J/molxK	482.04	Joback Method
cpg	190.43	J/molxK	516.72	Joback Method
cpg	197.67	J/molxK	551.41	Joback Method
cpg	204.52	J/molxK	586.09	Joback Method
cpg	210.99	J/molxK	620.77	Joback Method
cpg	217.11	J/molxK	655.45	Joback Method

Sources

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=C5414211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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