

Propanenitrile, 3-bromo-

Other names:	Propionitrile, 3-bromo- «beta»-Bromopropionitrile 1-Bromo-2-cyanoethane 2-Bromoethyl cyanide 3-Bromopropionitrile USAF DO-51 2-Cyanoethyl bromide Propionitrile, «beta»-bromo- NSC 8021 3-bromopropiononitrile
Inchi:	InChI=1S/C3H4BrN/c4-2-1-3-5/h1-2H2
InchiKey:	CQZIEDXCLQOOEH-UHFFFAOYSA-N
Formula:	C3H4BrN
SMILES:	N#CCCB
Mol. weight [g/mol]:	133.97
CAS:	2417-90-5

Physical Properties

Property code	Value	Unit	Source
gf	121.88	kJ/mol	Joback Method
hf	85.96	kJ/mol	Joback Method
hfus	10.32	kJ/mol	Joback Method
hvap	39.19	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.295		Crippen Method
mcvol	72.010	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	436.28	K	Joback Method
tc	650.16	K	Joback Method
tf	248.36	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.69	J/mol×K	436.28	Joback Method
cpg	114.36	J/mol×K	471.93	Joback Method
cpg	118.75	J/mol×K	507.57	Joback Method
cpg	122.89	J/mol×K	543.22	Joback Method
cpg	126.80	J/mol×K	578.87	Joback Method
cpg	130.47	J/mol×K	614.51	Joback Method
cpg	133.93	J/mol×K	650.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	1.30	NIST Webbook

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=C2417905&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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