2-Bromoacetamide

Other names: Acetamide, 2-bromo-
Bromoacetamide
Inchi: InChI=1S/C2H4BrNO/c3-1-2(4)5/h1H2,(H2,4,5)
InchiKey: JUIKUQOUMZUFQT-UHFFFAOYSA-N
Formula: C2H4BrNO
SMILES: NC(=O)CBr
Mol. weight [g/mol]: 137.96
CAS: 683-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-82.19	kJ/mol	Joback Method
hf	-137.07	kJ/mol	Joback Method
hfus	13.02	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
log10ws	-0.30		Crippen Method
logp	-0.133		Crippen Method
mcvol	68.090	ml/mol	McGowan Method
pc	6707.62	kPa	Joback Method
tb	437.72	K	Joback Method
tc	656.98	K	Joback Method
tf	305.29	K	Joback Method
vc	0.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.88	J/mol×K	437.72	Joback Method
cpg	113.67	J/mol×K	474.26	Joback Method
cpg	118.17	J/mol×K	510.81	Joback Method
cpg	122.37	J/mol×K	547.35	Joback Method
cpg	126.31	J/mol×K	583.89	Joback Method
cpg	129.99	J/mol×K	620.44	Joback Method
cpg	133.43	J/mol×K	656.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C683578&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume