Bromacetamide, N-(3-methylbutyl)-

Inchi: InChI=1S/C7H14BrNO/c1-6(2)3-4-9-7(10)5-8/h6H,3-5H2,1-2H3,(H,9,10)
InchiKey: HSFWFNUAKKZHOW-UHFFFAOYSA-N
Formula: C7H14BrNO
SMILES: CC(C)CCNC(=O)CBr
Mol. weight [g/mol]: 208.10

Physical Properties

Property code	Value	Unit	Source
gf	-19.59	kJ/mol	Joback Method
hf	-225.87	kJ/mol	Joback Method
hfus	22.35	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.544		Crippen Method
mcvol	138.540	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
tb	529.32	K	Joback Method
tc	728.52	K	Joback Method
tf	316.04	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.66	J/mol×K	529.32	Joback Method
cpg	310.38	J/mol×K	562.52	Joback Method
cpg	321.49	J/mol×K	595.72	Joback Method
cpg	332.00	J/mol×K	628.92	Joback Method
cpg	341.93	J/mol×K	662.12	Joback Method
cpg	351.32	J/mol×K	695.32	Joback Method
cpg	360.19	J/mol×K	728.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407073&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume