Hexanoic acid, 2-bromo-

Other names:	«alpha»-Bromo-n-caproic acid
	«alpha»-Bromocaproic acid
	«alpha»-Bromohexanoic acid
	2-Bromocaproic acid
	2-Bromohexanoic acid
Inchi:	InChI=1S/C6H11BrO2/c1-2-3-4-5(7)6(8)9/h5H,2-4H2,1H3,(H,8,9)
InchiKey:	HZTPKMIMXLTOSK-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CCCCC(Br)C(=O)O
Mol. weight [g/mol]:	195.05
CAS:	616-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-254.22	kJ/mol	Joback Method
hf	-410.93	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.025		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	548.45	K	Joback Method
tc	737.20	K	Joback Method
tf	312.93	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.40	J/mol×K	548.45	Joback Method
cpg	296.46	J/mol×K	705.74	Joback Method
cpg	289.46	J/mol×K	674.29	Joback Method
cpg	282.08	J/mol×K	642.83	Joback Method

cpg	274.29	J/mol×K	611.37	Joback Method
cpg	266.07	J/mol×K	579.91	Joback Method
cpg	303.08	J/mol×K	737.20	Joback Method
dvisc	0.0001610	Pa×s	548.45	Joback Method
dvisc	0.0002512	Pa×s	509.20	Joback Method
dvisc	0.0004220	Pa×s	469.94	Joback Method
dvisc	0.0007795	Pa×s	430.69	Joback Method
dvisc	0.0016283	Pa×s	391.44	Joback Method
dvisc	0.0040083	Pa×s	352.18	Joback Method
dvisc	0.0123694	Pa×s	312.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	2.40	NIST Webbook

Sources

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=C616057&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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