Hexanoic acid, 6-bromo-

Other names:	6-Bromohexanoic acid
	6-Bromocaproic acid
	6-Bromo-n-caproic acid
Inchi:	InChI=1S/C6H11BrO2/c7-5-3-1-2-4-6(8)9/h1-5H2,(H,8,9)
InchiKey:	NVRVNSHHLPQGCU-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	O=C(O)CCCCCBr
Mol. weight [g/mol]:	195.05
CAS:	4224-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-251.78	kJ/mol	Joback Method
hf	-405.65	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	2.026		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	548.89	K	Joback Method
tc	733.96	K	Joback Method
tf	327.93	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.01	J/mol×K	548.89	Joback Method
cpg	265.44	J/mol×K	579.73	Joback Method
cpg	273.46	J/mol×K	610.58	Joback Method
cpg	281.07	J/mol×K	641.42	Joback Method
cpg	288.30	J/mol×K	672.27	Joback Method
cpg	295.16	J/mol×K	703.11	Joback Method

cpg	301.67	J/mol×K	733.96	Joback Method
dvisc	0.0079363	Pa×s	327.93	Joback Method
dvisc	0.0030314	Pa×s	364.76	Joback Method
dvisc	0.0013814	Pa×s	401.58	Joback Method
dvisc	0.0007184	Pa×s	438.41	Joback Method
dvisc	0.0004134	Pa×s	475.24	Joback Method
dvisc	0.0002576	Pa×s	512.06	Joback Method
dvisc	0.0001710	Pa×s	548.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.70	K	2.70	NIST Webbook

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=C4224708&Units=SI

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

Latest version available from:

https://www.chemeo.com/cid/98-536-9/Hexanoic-acid-6-bromo.pdf

Generated by Cheméo on 2024-10-12 09:00:15.367184515 +0000 UTC m=+3304478.004153763.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.