

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)CCCCBr
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/molxK	548.89	Joback Method
cpg	265.44	J/molxK	579.73	Joback Method
cpg	273.46	J/molxK	610.58	Joback Method
cpg	281.07	J/molxK	641.42	Joback Method
cpg	288.30	J/molxK	672.27	Joback Method
cpg	295.16	J/molxK	703.11	Joback Method

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

Pressure Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4224708&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

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

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