

2-Bromovaleric acid

Other names:	«alpha»-Bromovaleric acid «alpha»-Bromo-n-valeric acid Pentanoic acid, 2-bromo- «alpha»-Bromopentanoic acid Valeric acid, «alpha»-bromo- Valeric acid, 2-bromo- 2-Bromopentanoic acid
Inchi:	InChI=1S/C5H9BrO2/c1-2-3-4(6)5(7)8/h4H,2-3H2,1H3,(H,7,8)
InchiKey:	WMFATTFQNRXPBQ-UHFFFAOYSA-N
Formula:	C5H9BrO2
SMILES:	CCCC(Br)C(=O)O
Mol. weight [g/mol]:	181.03
CAS:	584-93-0

Physical Properties

Property code	Value	Unit	Source
gf	-262.64	kJ/mol	Joback Method
hf	-390.29	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.635		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	525.57	K	Joback Method
tc	716.62	K	Joback Method
tf	301.66	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.09	J/molxK	525.57	Joback Method
cpg	222.71	J/molxK	557.41	Joback Method

cpg	229.94	J/molxK	589.25	Joback Method
cpg	236.78	J/molxK	621.10	Joback Method
cpg	243.26	J/molxK	652.94	Joback Method
cpg	249.38	J/molxK	684.78	Joback Method
cpg	255.18	J/molxK	716.62	Joback Method
dvisc	0.0149569	Paxs	301.66	Joback Method
dvisc	0.0048789	Paxs	338.98	Joback Method
dvisc	0.0019875	Paxs	376.30	Joback Method
dvisc	0.0009520	Paxs	413.62	Joback Method
dvisc	0.0005151	Paxs	450.93	Joback Method
dvisc	0.0003062	Paxs	488.25	Joback Method
dvisc	0.0001959	Paxs	525.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.20	K	3.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C584930&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
hvac:	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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