2-Bromobutyric acid

Other names:	«alpha»-Bromobytyric acid
	«alpha»-Bromo-n-butyric acid
	Butanoic acid, 2-bromo-
	Butyric acid, «alpha»-bromo-
	Butyric acid, 2-bromo-
	2-Bromobutanoic acid
	dl-2-Bromobutyric acid
Inchi:	InChI=1S/C4H7BrO2/c1-2-3(5)4(6)7/h3H,2H2,1H3,(H,6,7)
InchiKey:	YAQLSKVCTLCIIE-UHFFFAOYSA-N
Formula:	C4H7BrO2
SMILES:	CCC(Br)C(=O)O
Mol. weight [g/mol]:	167.00
CAS:	80-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-271.06	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.244		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	502.69	K	Joback Method
tc	696.12	K	Joback Method
tf	290.39	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.75	J/mol×K	502.69	Joback Method
cpg	181.21	J/mol×K	534.93	Joback Method

cpg	187.32	J/mol×K	567.17	Joback Method
cpg	193.11	J/mol×K	599.41	Joback Method
cpg	198.57	J/mol×K	631.65	Joback Method
cpg	203.74	J/mol×K	663.89	Joback Method
cpg	208.61	J/mol×K	696.12	Joback Method
dvisc	0.0180688	Pa×s	290.39	Joback Method
dvisc	0.0059375	Pa×s	325.77	Joback Method
dvisc	0.0024265	Pa×s	361.16	Joback Method
dvisc	0.0011634	Pa×s	396.54	Joback Method
dvisc	0.0006292	Pa×s	431.92	Joback Method
dvisc	0.0003734	Pa×s	467.31	Joback Method
dvisc	0.0002386	Pa×s	502.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	374.20	K	1.30	NIST Webbook
tbrp	364.50 ± 1.50	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80580&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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