Butanoic acid, 2-bromo-3-methyl-

Other names:	Butyric acid, 2-bromo-3-methyl-
	«alpha»-Bromoisovaleric acid
	2-Bromo-3-methylbutyric acid
	2-Bromoisovaleric acid
	2-Bromo-3-methylbutanoic acid
	NSC 167
	Isovaleric acid, «alpha»-bromo-
Inchi:	InChI=1S/C5H9BrO2/c1-3(2)4(6)5(7)8/h3-4H,1-2H3,(H,7,8)
InchiKey:	UEBARDWJXBGYEJ-UHFFFAOYSA-N
Formula:	C5H9BrO2
SMILES:	CC(C)C(Br)C(=O)O
Mol. weight [g/mol]:	181.03
CAS:	565-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-265.08	kJ/mol	Joback Method
hf	-395.57	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.490		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	525.13	K	Joback Method
tc	720.21	K	Joback Method
tf	286.66	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.45	J/mol×K	525.13	Joback Method
cpg	250.64	J/mol×K	687.70	Joback Method

cpg	244.38	J/mol×K	655.19	Joback Method
cpg	237.75	J/mol×K	622.67	Joback Method
cpg	230.73	J/mol×K	590.16	Joback Method
cpg	223.30	J/mol×K	557.64	Joback Method
cpg	256.54	J/mol×K	720.21	Joback Method
dvisc	0.0001851	Pa×s	525.13	Joback Method
dvisc	0.0003004	Pa×s	485.38	Joback Method
dvisc	0.0005317	Pa×s	445.64	Joback Method
dvisc	0.0010525	Pa×s	405.89	Joback Method
dvisc	0.0024162	Pa×s	366.15	Joback Method
dvisc	0.0067911	Pa×s	326.41	Joback Method
dvisc	0.0254209	Pa×s	286.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	2.70	NIST Webbook

Sources

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=C565742&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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