«alpha»-Bromoisobutyric acid

Other names:	2-Bromoisobutyric acid 2-Bromo-2-methylpropionic acid Propanoic acid, 2-bromo-2-methyl- Isobromobutyric acid Propionic acid, 2-bromo-2-methyl- 2-Bromo-2-methylpropanoic acid
Inchi:	InChI=1S/C4H7BrO2/c1-4(2,5)3(6)7/h1-2H3,(H,6,7)
InchiKey:	XXSPGBOGLXKMDU-UHFFFAOYSA-N
Formula:	C4H7BrO2
SMILES:	CC(C)(Br)C(=O)O
Mol. weight [g/mol]:	167.00
CAS:	2052-01-9

Physical Properties

Property code	Value	Unit	Source
gf	-265.78	kJ/mol	Joback Method
hf	-373.12	kJ/mol	Joback Method
hfus	9.67	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.244		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
tb	472.20	K	NIST Webbook
tc	701.13	K	Joback Method
tf	307.81	K	Joback Method
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.24	J/mol×K	499.90	Joback Method
cpg	207.98	J/mol×K	667.59	Joback Method
cpg	202.89	J/mol×K	634.05	Joback Method

cpg	197.40	J/mol×K	600.51	Joback Method
cpg	191.49	J/mol×K	566.98	Joback Method
cpg	185.11	J/mol×K	533.44	Joback Method
cpg	212.70	J/mol×K	701.13	Joback Method
dvisc	0.0002479	Pa×s	499.90	Joback Method
dvisc	0.0003831	Pa×s	467.88	Joback Method
dvisc	0.0006309	Pa×s	435.87	Joback Method
dvisc	0.0011245	Pa×s	403.86	Joback Method
dvisc	0.0022143	Pa×s	371.84	Joback Method
dvisc	0.0049538	Pa×s	339.82	Joback Method
dvisc	0.0131037	Pa×s	307.81	Joback Method

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=C2052019&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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