3-BROMOBUTYRIC ACID

Other names: Butanoic acid, 3-bromo-
Inchi: InChI=1S/C4H7BrO2/c1-3(5)2-4(6)7/h3H,2H2,1H3,(H,6,7)
InchiKey: HAIUIAZIUDPZIE-UHFFFAOYSA-N
Formula: C4H7BrO2
SMILES: CC(Br)CC(=O)O
Mol. weight [g/mol]: 167.00

Physical Properties

Property code	Value	Unit	Source
hf	-471.57	kJ/mol	Cheméo Relay (1.0)
hfus	13.56	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Cheméo Relay (1.0)
ie	10.35	eV	Cheméo Relay (1.0)
log10ws	-0.40		Cheméo Relay (1.0)
logp	1.244		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	476.95	K	Cheméo Relay (1.0)
tc	686.51	K	Cheméo Relay (1.0)
tf	322.14	K	Cheméo Relay (1.0)

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	395.00	K	2.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623861&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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

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