4-BROMOBUTYRIC ACID

Other names:	4-Bromo-n-butyric acid
	Butanoic acid, 4-bromo-
	Butyric acid, 4-bromo-
	4-Bromobutanoic acid
	«gamma»-Bromobutyric acid
	Carboxypropyl bromide
Inchi:	InChI=1S/C4H7BrO2/c5-3-1-2-4(6)7/h1-3H2,(H,6,7)
InchiKey:	GRHQDJDRGZFIPO-UHFFFAOYSA-N
Formula:	C4H7BrO2
SMILES:	O=C(O)CCCBr
Mol. weight [g/mol]:	167.00

Physical Properties

Property code	Value	Unit	Source
af	0.6990		Cheméo Relay (1.0)
gf	-268.62	kJ/mol	Joback Method
hf	-448.67	kJ/mol	Cheméo Relay (1.0)
hfus	17.09	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Cheméo Relay (1.0)
ie	10.37	eV	Cheméo Relay (1.0)
log10ws	-0.51		Cheméo Relay (1.0)
logp	1.246		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	5266.25	kPa	Joback Method
tb	513.06	K	Cheméo Relay (1.0)
tc	710.09	K	Cheméo Relay (1.0)
tf	306.00	K	NIST Webbook
vc	0.319	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.41	J/mol×K	503.13	Joback Method
cpg	207.36	J/mol×K	692.48	Joback Method

cpg	202.59	J/mol×K	660.92	Joback Method
cpg	197.54	J/mol×K	629.36	Joback Method
cpg	192.22	J/mol×K	597.80	Joback Method
cpg	186.60	J/mol×K	566.25	Joback Method
cpg	180.67	J/mol×K	534.69	Joback Method
dvisc	0.0010497	Pa×s	404.26	Joback Method
dvisc	0.0002517	Pa×s	503.13	Joback Method
dvisc	0.0003790	Pa×s	470.17	Joback Method
dvisc	0.0006070	Pa×s	437.22	Joback Method
dvisc	0.0110350	Pa×s	305.39	Joback Method
dvisc	0.0020006	Pa×s	371.30	Joback Method
dvisc	0.0043236	Pa×s	338.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.70	K	1.50	NIST Webbook
tbrp	381.50 ± 0.50	K	0.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623872&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

af: Acentric Factor
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
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
vc:	Critical Volume