

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)CCCB
Mol. weight [g/mol]:	167.00
CAS:	2623-87-2

Physical Properties

Property code	Value	Unit	Source
gf	-268.62	kJ/mol	Joback Method
hf	-364.37	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	54.36	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	1.246		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	5266.25	kPa	Joback Method
tb	503.13	K	Joback Method
tc	692.48	K	Joback Method
tf	306.00	K	NIST Webbook
vc	0.346	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.41	J/mol×K	503.13	Joback Method
cpg	180.67	J/mol×K	534.69	Joback Method
cpg	186.60	J/mol×K	566.25	Joback Method

cpg	192.22	J/mol×K	597.80	Joback Method
cpg	197.54	J/mol×K	629.36	Joback Method
cpg	202.59	J/mol×K	660.92	Joback Method
cpg	207.36	J/mol×K	692.48	Joback Method
dvisc	0.0110350	Paxs	305.39	Joback Method
dvisc	0.0043236	Paxs	338.35	Joback Method
dvisc	0.0020006	Paxs	371.30	Joback Method
dvisc	0.0010497	Paxs	404.26	Joback Method
dvisc	0.0006070	Paxs	437.22	Joback Method
dvisc	0.0003790	Paxs	470.17	Joback Method
dvisc	0.0002517	Paxs	503.13	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

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=C2623872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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