1-Butanol, 4-bromo-

Other names: 4-Bromo-1-butanol
4-bromobutan-1-ol
Inchi: InChI=1S/C4H9BrO/c5-3-1-2-4-6/h6H,1-4H2
InchiKey: SIJLYRDVTMMSIP-UHFFFAOYSA-N
Formula: C4H9BrO
SMILES: OCCCCBr
Mol. weight [g/mol]: 153.02
CAS: 33036-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-139.70	kJ/mol	Joback Method
hf	-251.79	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	47.61	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.154		Crippen Method
mcvol	90.590	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	449.26	K	Joback Method
tc	628.58	K	Joback Method
tf	255.46	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.22	J/mol×K	449.26	Joback Method
cpg	197.02	J/mol×K	598.69	Joback Method
cpg	191.25	J/mol×K	568.80	Joback Method
cpg	185.20	J/mol×K	538.92	Joback Method
cpg	178.85	J/mol×K	509.03	Joback Method
cpg	172.19	J/mol×K	479.15	Joback Method
cpg	202.51	J/mol×K	628.58	Joback Method

dvisc	0.0003123	Pa×s	449.26	Joback Method
dvisc	0.0004967	Pa×s	416.96	Joback Method
dvisc	0.0008541	Pa×s	384.66	Joback Method
dvisc	0.0016220	Pa×s	352.36	Joback Method
dvisc	0.0035062	Pa×s	320.06	Joback Method
dvisc	0.0090108	Pa×s	287.76	Joback Method
dvisc	0.0294007	Pa×s	255.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.00 ± 1.00	K	0.30	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=C33036623&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