

1-Butanol, 4-bromo-, acetate

Other names:	4-Bromo-n-butyl acetate 4-Bromobutyl acetate
Inchi:	InChI=1S/C6H11BrO2/c1-6(8)9-5-3-2-4-7/h2-5H2,1H3
InchiKey:	UOABIRUEGSGTSA-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CC(=O)OCCCCBr
Mol. weight [g/mol]:	195.05
CAS:	4753-59-7

Physical Properties

Property code	Value	Unit	Source
gf	-219.96	kJ/mol	Joback Method
hf	-385.64	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.725		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	479.13	K	Joback Method
tc	673.53	K	Joback Method
tf	289.34	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.29	J/mol×K	479.13	Joback Method
cpg	245.05	J/mol×K	511.53	Joback Method
cpg	254.40	J/mol×K	543.93	Joback Method
cpg	263.33	J/mol×K	576.33	Joback Method
cpg	271.87	J/mol×K	608.73	Joback Method
cpg	280.00	J/mol×K	641.13	Joback Method
cpg	287.75	J/mol×K	673.53	Joback Method

dvisc	0.0026449	Pa×s	289.34	Joback Method
dvisc	0.0015715	Pa×s	320.97	Joback Method
dvisc	0.0010251	Pa×s	352.60	Joback Method
dvisc	0.0007175	Pa×s	384.24	Joback Method
dvisc	0.0005301	Pa×s	415.87	Joback Method
dvisc	0.0004089	Pa×s	447.50	Joback Method
dvisc	0.0003263	Pa×s	479.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4753597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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