

1-Bromo-3-butene-2-ol

Other names:	1-Bromo-3-buten-2-ol
Inchi:	InChI=1S/C4H7BrO/c1-2-4(6)3-5/h2,4,6H,1,3H2
InchiKey:	PDAWHBQDMPNZQI-UHFFFAOYSA-N
Formula:	C4H7BrO
SMILES:	C=CC(O)CBr
Mol. weight [g/mol]:	151.00
CAS:	64341-49-7

Physical Properties

Property code	Value	Unit	Source
gf	-54.30	kJ/mol	Joback Method
hf	-131.64	kJ/mol	Joback Method
hfus	10.69	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	0.928		Crippen Method
mcvol	86.290	ml/mol	McGowan Method
pc	5168.28	kPa	Joback Method
tb	445.50	K	Joback Method
tc	632.65	K	Joback Method
tf	238.70	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.67	J/mol×K	445.50	Joback Method
cpg	156.14	J/mol×K	476.69	Joback Method
cpg	162.25	J/mol×K	507.88	Joback Method
cpg	168.02	J/mol×K	539.08	Joback Method
cpg	173.47	J/mol×K	570.27	Joback Method
cpg	178.62	J/mol×K	601.46	Joback Method
cpg	183.48	J/mol×K	632.65	Joback Method
dvisc	0.0543785	Pa×s	238.70	Joback Method

dvisc	0.0132998	Pa×s	273.17	Joback Method
dvisc	0.0044597	Pa×s	307.63	Joback Method
dvisc	0.0018637	Pa×s	342.10	Joback Method
dvisc	0.0009137	Pa×s	376.57	Joback Method
dvisc	0.0005049	Pa×s	411.03	Joback Method
dvisc	0.0003058	Pa×s	445.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.00 ± 2.00	K	2.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64341497&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

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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