3-BUTEN-2-OL, 1-BROMO-

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

Physical Properties

Property code	Value	Unit	Source
hfus	10.69	kJ/mol	Joback Method
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-0.09		Cheméo Relay (1.0)
logp	0.928		Crippen Method
mcvol	86.290	ml/mol	McGowan Method
tb	431.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.67	J/mol×K	445.50	Joback Method
cpg	183.48	J/mol×K	632.65	Joback Method
cpg	178.62	J/mol×K	601.46	Joback Method
cpg	173.47	J/mol×K	570.27	Joback Method
cpg	168.02	J/mol×K	539.08	Joback Method
cpg	162.25	J/mol×K	507.88	Joback Method
cpg	156.14	J/mol×K	476.69	Joback Method
dvisc	0.0018637	Pa×s	342.10	Joback Method
dvisc	0.0003058	Pa×s	445.50	Joback Method
dvisc	0.0005049	Pa×s	411.03	Joback Method
dvisc	0.0009137	Pa×s	376.57	Joback Method
dvisc	0.0543785	Pa×s	238.70	Joback Method
dvisc	0.0044597	Pa×s	307.63	Joback Method
dvisc	0.0132998	Pa×s	273.17	Joback Method

Pressure Dependent Properties

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

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64341497&Units=SI
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
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure