

2-Propanol, 1-bromo-

Other names:	1-Bromo-2-propanol 2-Hydroxy-2-methylethyl bromide 2-Hydroxypropyl bromide Propylene bromohydrin 1-Bromo-2-hydroxypropane 1-bromopropan-2-ol
Inchi:	InChI=1S/C3H7BrO/c1-3(5)2-4/h3,5H,2H2,1H3
InchiKey:	WEGOLYBUWCMMMY-UHFFFAOYSA-N
Formula:	C3H7BrO
SMILES:	CC(O)CBr
Mol. weight [g/mol]:	138.99
CAS:	19686-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-150.56	kJ/mol	Joback Method
hf	-236.43	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	45.00	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.762		Crippen Method
mcvol	76.500	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
tb	419.70	K	NIST Webbook
tc	610.84	K	Joback Method
tf	229.19	K	Joback Method
vc	0.279	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.15	J/mol×K	425.94	Joback Method
cpg	135.04	J/mol×K	456.76	Joback Method
cpg	140.63	J/mol×K	487.57	Joback Method

cpg	145.95	J/molxK	518.39	Joback Method
cpg	151.01	J/molxK	549.21	Joback Method
cpg	155.81	J/molxK	580.03	Joback Method
cpg	160.37	J/molxK	610.84	Joback Method
dvisc	0.0745644	Paxs	229.19	Joback Method
dvisc	0.0176820	Paxs	261.98	Joback Method
dvisc	0.0057755	Paxs	294.77	Joback Method
dvisc	0.0023601	Paxs	327.56	Joback Method
dvisc	0.0011351	Paxs	360.36	Joback Method
dvisc	0.0006168	Paxs	393.15	Joback Method
dvisc	0.0003682	Paxs	425.94	Joback Method

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=C19686738&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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