

1-Propanol, 3-bromo-

Other names:	Trimethylene bromohydrin 1-Bromo-3-propanol 3-Bromo-1-propanol 3-Hydroxypropyl bromide 3-Bromopropanol-(1) 3-Bromopropanol 1-Bromo-3-hydroxypropane 3-bromopropan-1-ol
Inchi:	InChI=1S/C3H7BrO/c4-2-1-3-5/h5H,1-3H2
InchiKey:	RQFUZUMFPRMVDX-UHFFFAOYSA-N
Formula:	C3H7BrO
SMILES:	OCCCB
Mol. weight [g/mol]:	138.99
CAS:	627-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-148.12	kJ/mol	Joback Method
hf	-231.15	kJ/mol	Joback Method
hfus	12.90	kJ/mol	Joback Method
hvap	45.39	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.764		Crippen Method
mcvol	76.500	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	426.38	K	Joback Method
tc	607.13	K	Joback Method
tf	244.19	K	Joback Method
vc	0.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.02	J/mol×K	426.38	Joback Method

cpg	134.68	J/molxK	456.50	Joback Method
cpg	140.08	J/molxK	486.63	Joback Method
cpg	145.22	J/molxK	516.75	Joback Method
cpg	150.12	J/molxK	546.88	Joback Method
cpg	154.78	J/molxK	577.00	Joback Method
cpg	159.22	J/molxK	607.13	Joback Method
dvisc	0.0360361	Paxs	244.19	Joback Method
dvisc	0.0111136	Paxs	274.56	Joback Method
dvisc	0.0043324	Paxs	304.92	Joback Method
dvisc	0.0020031	Paxs	335.28	Joback Method
dvisc	0.0010527	Paxs	365.65	Joback Method
dvisc	0.0006106	Paxs	396.01	Joback Method
dvisc	0.0003828	Paxs	426.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	0.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627189&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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