

3-Bromo-1,2-propanediol

Other names:	1,2-Propanediol, 3-bromo- 3-Bromodeoxyglycerol «alpha»-Bromohydrin Monobromoglycerol 3-bromopropane-1,2-diol
Inchi:	InChI=1S/C3H7BrO2/c4-1-3(6)2-5/h3,5-6H,1-2H2
InchiKey:	SIBFQOUHOCRXDL-UHFFFAOYSA-N
Formula:	C3H7BrO2
SMILES:	OCC(O)CBr
Mol. weight [g/mol]:	154.99
CAS:	4704-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-287.38	kJ/mol	Joback Method
hf	-388.66	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.265		Crippen Method
mcvol	82.370	ml/mol	McGowan Method
pc	6451.51	kPa	Joback Method
tb	518.12	K	Joback Method
tc	694.88	K	Joback Method
tf	290.01	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.00	J/mol×K	518.12	Joback Method
cpg	167.14	J/mol×K	547.58	Joback Method
cpg	172.02	J/mol×K	577.04	Joback Method
cpg	176.65	J/mol×K	606.50	Joback Method

cpg	181.05	J/mol×K	635.96	Joback Method
cpg	185.24	J/mol×K	665.42	Joback Method
cpg	189.21	J/mol×K	694.88	Joback Method
dvisc	0.0815985	Pa×s	290.01	Joback Method
dvisc	0.0143177	Pa×s	328.03	Joback Method
dvisc	0.0036063	Pa×s	366.05	Joback Method
dvisc	0.0011774	Pa×s	404.06	Joback Method
dvisc	0.0004660	Pa×s	442.08	Joback Method
dvisc	0.0002136	Pa×s	480.10	Joback Method
dvisc	0.0001098	Pa×s	518.12	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.70	K	0.03	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4704772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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