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

Physical Properties

Property code	Value	Unit	Source
hf	-432.61	kJ/mol	Cheméo Relay (1.0)
hfus	13.46	kJ/mol	Joback Method
hvap	82.38	kJ/mol	Cheméo Relay (1.0)
log10ws	0.64		Cheméo Relay (1.0)
logp	-0.265		Crippen Method
mcvol	82.370	ml/mol	McGowan Method
pc	6451.51	kPa	Joback Method
tb	517.25	K	Cheméo Relay (1.0)
tc	753.51	K	Cheméo Relay (1.0)
tf	264.05	K	Cheméo Relay (1.0)
vc	0.297	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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=C4704772&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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