1-Bromo-2,2-dimethoxypropane

Other names: Propane, 1-bromo-2,2-dimethoxy-
Inchi: InChI=1S/C5H11BrO2/c1-5(4-6,7-2)8-3/h4H2,1-3H3
InchiKey: SGTITUFGCGGICE-UHFFFAOYSA-N
Formula: C5H11BrO2
SMILES: COC(C)(CBr)OC
Mol. weight [g/mol]: 183.04
CAS: 126-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-201.62	kJ/mol	Joback Method
hf	-393.39	kJ/mol	Joback Method
hfus	8.95	kJ/mol	Joback Method
hvap	36.68	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.390		Crippen Method
mcvol	110.550	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	421.57	K	Joback Method
tc	618.50	K	Joback Method
tf	252.79	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.26	J/mol×K	421.57	Joback Method
cpg	216.31	J/mol×K	454.39	Joback Method
cpg	225.91	J/mol×K	487.21	Joback Method
cpg	235.07	J/mol×K	520.03	Joback Method
cpg	243.80	J/mol×K	552.86	Joback Method
cpg	252.11	J/mol×K	585.68	Joback Method
cpg	260.01	J/mol×K	618.50	Joback Method
dvisc	0.0032903	Pa×s	252.79	Joback Method

dvisc	0.0017802	Pa×s	280.92	Joback Method
dvisc	0.0010771	Pa×s	309.05	Joback Method
dvisc	0.0007087	Pa×s	337.18	Joback Method
dvisc	0.0004973	Pa×s	365.31	Joback Method
dvisc	0.0003671	Pa×s	393.44	Joback Method
dvisc	0.0002822	Pa×s	421.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	11.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C126385&Units=SI

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