3-Bromopropionaldehyde dimethyl acetal

Other names: Propane, 3-bromo-1,1-dimethoxy-
3-bromo-1,1-dimethoxypropane
Inchi: InChI=1S/C5H11BrO2/c1-7-5(8-2)3-4-6/h5H,3-4H2,1-2H3
InchiKey: ODZZAIFAQLODKN-UHFFFAOYSA-N
Formula: C5H11BrO2
SMILES: COC(CCBr)OC
Mol. weight [g/mol]: 183.04
CAS: 36255-44-4

Physical Properties

Property code	Value	Unit	Source
gf	-206.90	kJ/mol	Joback Method
hf	-389.92	kJ/mol	Joback Method
hfus	12.84	kJ/mol	Joback Method
hvap	37.59	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.390		Crippen Method
mcvol	110.550	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	424.36	K	Joback Method
tc	613.19	K	Joback Method
tf	235.37	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.86	J/mol×K	424.36	Joback Method
cpg	213.04	J/mol×K	455.83	Joback Method
cpg	221.95	J/mol×K	487.30	Joback Method
cpg	230.57	J/mol×K	518.77	Joback Method
cpg	238.91	J/mol×K	550.24	Joback Method
cpg	246.96	J/mol×K	581.72	Joback Method
cpg	254.72	J/mol×K	613.19	Joback Method

dvisc	0.0032665	Pa×s	235.37	Joback Method
dvisc	0.0016615	Pa×s	266.87	Joback Method
dvisc	0.0009748	Pa×s	298.37	Joback Method
dvisc	0.0006332	Pa×s	329.87	Joback Method
dvisc	0.0004435	Pa×s	361.36	Joback Method
dvisc	0.0003288	Pa×s	392.86	Joback Method
dvisc	0.0002549	Pa×s	424.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	2.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36255444&Units=SI
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

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