3-Bromo-2,2-dimethyl-1-propanol

Inchi: InChI=1S/C5H11BrO/c1-5(2,3-6)4-7/h7H,3-4H2,1-2H3
InchiKey: KQOQXYPZBYTICM-UHFFFAOYSA-N
Formula: C5H11BrO
SMILES: CC(C)(CO)CBr
Mol. weight [g/mol]: 167.04
CAS: 40894-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-128.44	kJ/mol	Joback Method
hf	-281.18	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.400		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	458.70	K	NIST Webbook
tc	657.78	K	Joback Method
tf	269.15	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.92	J/mol×K	468.91	Joback Method
cpg	215.94	J/mol×K	500.39	Joback Method
cpg	224.42	J/mol×K	531.87	Joback Method
cpg	232.39	J/mol×K	563.35	Joback Method
cpg	239.87	J/mol×K	594.83	Joback Method
cpg	246.89	J/mol×K	626.30	Joback Method
cpg	253.50	J/mol×K	657.78	Joback Method
dvisc	0.0312926	Pa×s	269.15	Joback Method
dvisc	0.0090766	Pa×s	302.44	Joback Method

dvisc	0.0033652	Pa×s	335.74	Joback Method
dvisc	0.0014923	Pa×s	369.03	Joback Method
dvisc	0.0007571	Pa×s	402.32	Joback Method
dvisc	0.0004261	Pa×s	435.62	Joback Method
dvisc	0.0002602	Pa×s	468.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40894006&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume