Propanoic acid, 3-bromo-

Other names:	Propionic acid, 3-bromo-
	«beta»-Bromopropionic acid
	2-Carboxyethyl bromide
	3-Bromopropanoic acid
	3-Bromopropionic acid
Inchi:	InChI=1S/C3H5BrO2/c4-2-1-3(5)6/h1-2H2,(H,5,6)
InchiKey:	DHXNZYCXMFBMHE-UHFFFAOYSA-N
Formula:	C3H5BrO2
SMILES:	O=C(O)CCBr
Mol. weight [g/mol]:	152.97
CAS:	590-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-277.04	kJ/mol	Joback Method
hf	-343.73	kJ/mol	Joback Method
hfus	14.50	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	0.856		Crippen Method
mcvol	78.070	ml/mol	McGowan Method
pc	6084.49	kPa	Joback Method
rinpol	1024.00		NIST Webbook
tb	480.25	K	Joback Method
tc	671.82	K	Joback Method
tf	294.12	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.18	J/mol×K	480.25	Joback Method
cpg	141.17	J/mol×K	512.18	Joback Method
cpg	145.88	J/mol×K	544.11	Joback Method

cpg	150.34	J/mol×K	576.03	Joback Method
cpg	154.55	J/mol×K	607.96	Joback Method
cpg	158.53	J/mol×K	639.89	Joback Method
cpg	162.29	J/mol×K	671.82	Joback Method
dvisc	0.0129460	Pa×s	294.12	Joback Method
dvisc	0.0051469	Pa×s	325.14	Joback Method
dvisc	0.0024029	Pa×s	356.16	Joback Method
dvisc	0.0012675	Pa×s	387.19	Joback Method
dvisc	0.0007351	Pa×s	418.21	Joback Method
dvisc	0.0004597	Pa×s	449.23	Joback Method
dvisc	0.0003054	Pa×s	480.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.20	K	6.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C590921&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume