Propanoic acid, 2-bromo-, (.+/-.)-

Inchi: InChI=1S/C3H5BrO2/c1-2(4)3(5)6/h2H,1H3,(H,5,6)
InchiKey: MONMFXREYOKQTI-UHFFFAOYSA-N
Formula: C3H5BrO2
SMILES: CC(Br)C(=O)O
Mol. weight [g/mol]: 152.97
CAS: 10327-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-279.48	kJ/mol	Joback Method
hf	-349.01	kJ/mol	Joback Method
hfus	10.97	kJ/mol	Joback Method
hvap	51.74	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.854		Crippen Method
mcvol	78.070	ml/mol	McGowan Method
pc	6161.14	kPa	Joback Method
tb	476.70	K	NIST Webbook
tc	675.66	K	Joback Method
tf	279.12	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.48	J/mol×K	479.81	Joback Method
cpg	141.65	J/mol×K	512.45	Joback Method
cpg	146.53	J/mol×K	545.09	Joback Method
cpg	151.14	J/mol×K	577.73	Joback Method
cpg	155.49	J/mol×K	610.37	Joback Method
cpg	159.58	J/mol×K	643.02	Joback Method
cpg	163.43	J/mol×K	675.66	Joback Method
dvisc	0.0217983	Pa×s	279.12	Joback Method
dvisc	0.0072223	Pa×s	312.57	Joback Method

dvisc	0.0029627	Pa×s	346.02	Joback Method
dvisc	0.0014220	Pa×s	379.47	Joback Method
dvisc	0.0007687	Pa×s	412.91	Joback Method
dvisc	0.0004557	Pa×s	446.36	Joback Method
dvisc	0.0002906	Pa×s	479.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10327089&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