Propanoic acid, 3-bromo-2-(bromomethyl)-

Other names:	«beta»,«beta»-Dibromoisobutyric acid
	Propionic acid, 3-bromo-2-(bromomethyl)-
	3-BROMO-2-(BROMOMETHYL)PROPIONIC ACID
Inchi:	InChI=1S/C4H6Br2O2/c5-1-3(2-6)4(7)8/h3H,1-2H2,(H,7,8)
InchiKey:	QQZJWQCLWOQDQV-UHFFFAOYSA-N
Formula:	C4H6Br2O2
SMILES:	O=C(O)C(CBr)CBr
Mol. weight [g/mol]:	245.90
CAS:	41459-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-256.74	kJ/mol	Joback Method
hf	-343.32	kJ/mol	Joback Method
hfus	18.85	kJ/mol	Joback Method
hvap	60.41	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.477		Crippen Method
mcvol	109.660	ml/mol	McGowan Method
pc	5908.07	kPa	Joback Method
tb	568.85	K	Joback Method
tc	776.12	K	Joback Method
tf	350.19	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.72	J/mol×K	568.85	Joback Method
cpg	226.16	J/mol×K	741.58	Joback Method
cpg	221.74	J/mol×K	707.03	Joback Method
cpg	217.01	J/mol×K	672.49	Joback Method
cpg	211.95	J/mol×K	637.94	Joback Method
cpg	206.53	J/mol×K	603.40	Joback Method

cpg	230.30	J/mol×K	776.12	Joback Method
dvisc	0.0001734	Pa×s	568.85	Joback Method
dvisc	0.0002567	Pa×s	532.41	Joback Method
dvisc	0.0004026	Pa×s	495.96	Joback Method
dvisc	0.0006781	Pa×s	459.52	Joback Method
dvisc	0.0012494	Pa×s	423.08	Joback Method
dvisc	0.0025833	Pa×s	386.63	Joback Method
dvisc	0.0062127	Pa×s	350.19	Joback Method

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=C41459421&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume