2-Propenoic acid, 2-bromoethyl ester

Other names: Acrylic acid, 2-bromoethyl ester
2-Bromoethyl acrylate
Inchi: InChI=1S/C5H7BrO2/c1-2-5(7)8-4-3-6/h2H,1,3-4H2
InchiKey: CDZAAIHWZYWBSS-UHFFFAOYSA-N
Formula: C5H7BrO2
SMILES: C=CC(=O)OCCBr
Mol. weight [g/mol]: 179.01
CAS: 4823-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-140.54	kJ/mol	Joback Method
hf	-239.57	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	41.64	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.110		Crippen Method
mcvol	101.950	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	452.93	K	Joback Method
tc	653.94	K	Joback Method
tf	276.31	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.89	J/mol×K	452.93	Joback Method
cpg	214.85	J/mol×K	620.44	Joback Method
cpg	208.54	J/mol×K	586.93	Joback Method
cpg	201.90	J/mol×K	553.43	Joback Method
cpg	194.92	J/mol×K	519.93	Joback Method
cpg	187.58	J/mol×K	486.43	Joback Method
cpg	220.83	J/mol×K	653.94	Joback Method

dvisc	0.0003545	Pa×s	452.93	Joback Method
dvisc	0.0004374	Pa×s	423.49	Joback Method
dvisc	0.0005569	Pa×s	394.06	Joback Method
dvisc	0.0007373	Pa×s	364.62	Joback Method
dvisc	0.0010253	Pa×s	335.18	Joback Method
dvisc	0.0015193	Pa×s	305.75	Joback Method
dvisc	0.0024481	Pa×s	276.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.00	K	0.70	NIST Webbook

Sources

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=C4823476&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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