2-Propenoic acid, 3-bromo-, methyl ester, (E)-

Inchi: InChI=1S/C4H5BrO2/c1-7-4(6)2-3-5/h2-3H,1H3/b3-2+
InchiKey: HGOGNLOBEAIJAM-NSCUHMNNSA-N
Formula: C4H5BrO2
SMILES: COC(=O)C=CBr
Mol. weight [g/mol]: 164.99
CAS: 6213-87-2

Physical Properties

Property code	Value	Unit	Source
gf	-156.58	kJ/mol	Joback Method
hf	-227.14	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	40.05	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.068		Crippen Method
mcvol	87.860	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	437.53	K	Joback Method
tc	646.70	K	Joback Method
tf	261.72	K	Joback Method
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.16	J/mol×K	437.53	Joback Method
cpg	148.61	J/mol×K	472.39	Joback Method
cpg	154.70	J/mol×K	507.25	Joback Method
cpg	160.47	J/mol×K	542.12	Joback Method
cpg	165.91	J/mol×K	576.98	Joback Method
cpg	171.05	J/mol×K	611.84	Joback Method
cpg	175.90	J/mol×K	646.70	Joback Method
dvisc	0.0023734	Pa×s	261.72	Joback Method
dvisc	0.0014304	Pa×s	291.02	Joback Method

dvisc	0.0009457	Pa×s	320.32	Joback Method
dvisc	0.0006701	Pa×s	349.62	Joback Method
dvisc	0.0005009	Pa×s	378.93	Joback Method
dvisc	0.0003903	Pa×s	408.23	Joback Method
dvisc	0.0003145	Pa×s	437.53	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=C6213872&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