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

Inchi: InChI=1S/C4H7BrO2/c1-3(5)4(6)7-2/h3H,1-2H3
InchiKey: ACEONLNNWKIPTM-UHFFFAOYSA-N
Formula: C4H7BrO2
SMILES: COC(=O)C(C)Br
Mol. weight [g/mol]: 167.00
CAS: 57885-43-5

Physical Properties

Property code	Value	Unit	Source
gf	-239.24	kJ/mol	Joback Method
hf	-349.64	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	39.70	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.943		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	417.20	K	NIST Webbook
tc	636.61	K	Joback Method
tf	251.80	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.91	J/mol×K	432.93	Joback Method
cpg	166.23	J/mol×K	466.88	Joback Method
cpg	173.25	J/mol×K	500.82	Joback Method
cpg	179.98	J/mol×K	534.77	Joback Method
cpg	186.40	J/mol×K	568.72	Joback Method
cpg	192.53	J/mol×K	602.66	Joback Method
cpg	198.37	J/mol×K	636.61	Joback Method
dvisc	0.0035651	Pa×s	251.80	Joback Method
dvisc	0.0019845	Pa×s	281.99	Joback Method

dvisc	0.0012371	Pa×s	312.18	Joback Method
dvisc	0.0008383	Pa×s	342.37	Joback Method
dvisc	0.0006050	Pa×s	372.55	Joback Method
dvisc	0.0004585	Pa×s	402.74	Joback Method
dvisc	0.0003612	Pa×s	432.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	324.70	K	2.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57885435&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

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