Propanoic acid, 2-bromo-, methyl ester

Other names:	Methyl «alpha»-bromopropionate
	Methyl dl-2-bromopropionate
	Methyl 2-bromopropanoate
	Methyl 2-bromopropionate
	Propionic acid, 2-bromo-, methyl ester
	2-Bromopropanoic acid methyl ester
	2-Bromopropionic acid 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:	5445-17-0

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
rinpol	838.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	836.00		NIST Webbook
tb	432.93	K	Joback Method
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	324.20	K	2.50	NIST Webbook

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=C5445170&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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