

# Propanoic acid, 2-bromo-, methyl ester

<b>Other names:</b>	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
<b>Inchi:</b>	InChI=1S/C4H7BrO2/c1-3(5)4(6)7-2/h3H,1-2H3
<b>InchiKey:</b>	ACEONLNNWKIPTM-UHFFFAOYSA-N
<b>Formula:</b>	C4H7BrO2
<b>SMILES:</b>	COC(=O)C(C)Br
<b>Mol. weight [g/mol]:</b>	167.00
<b>CAS:</b>	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	824.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		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/molxK	432.93	Joback Method
cpg	166.23	J/molxK	466.88	Joback Method
cpg	173.25	J/molxK	500.82	Joback Method
cpg	179.98	J/molxK	534.77	Joback Method
cpg	186.40	J/molxK	568.72	Joback Method
cpg	192.53	J/molxK	602.66	Joback Method
cpg	198.37	J/molxK	636.61	Joback Method
dvisc	0.0035651	Paxs	251.80	Joback Method
dvisc	0.0019845	Paxs	281.99	Joback Method
dvisc	0.0012371	Paxs	312.18	Joback Method
dvisc	0.0008383	Paxs	342.37	Joback Method
dvisc	0.0006050	Paxs	372.55	Joback Method
dvisc	0.0004585	Paxs	402.74	Joback Method
dvisc	0.0003612	Paxs	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:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/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>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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