

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

Other names:	Methyl (2Z)-3-bromo-2-propenoate
Inchi:	InChI=1S/C4H5BrO2/c1-7-4(6)2-3-5/h2-3H,1H3/b3-2-
InchiKey:	HGOGNLOBEAIJAM-IHWYPQMZSA-N
Formula:	C4H5BrO2
SMILES:	COC(=O)C=CBr
Mol. weight [g/mol]:	164.99
CAS:	6214-22-8

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/molxK	437.53	Joback Method
cpg	171.05	J/molxK	611.84	Joback Method
cpg	165.91	J/molxK	576.98	Joback Method
cpg	160.47	J/molxK	542.12	Joback Method
cpg	154.70	J/molxK	507.25	Joback Method
cpg	148.61	J/molxK	472.39	Joback Method
cpg	175.90	J/molxK	646.70	Joback Method
dvisc	0.0003145	Paxs	437.53	Joback Method

dvisc	0.0003903	Paxs	408.23	Joback Method
dvisc	0.0005009	Paxs	378.93	Joback Method
dvisc	0.0006701	Paxs	349.62	Joback Method
dvisc	0.0009457	Paxs	320.32	Joback Method
dvisc	0.0014304	Paxs	291.02	Joback Method
dvisc	0.0023734	Paxs	261.72	Joback Method

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=C6214228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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