Methyl 2,3-dibromopropionate

Other names:	Methyl «alpha»,«beta»-dibromopropionate
	Propanoic acid, 2,3-dibromo-, methyl ester
	Methyl dibromopropionate
	Methyl 2,3-dibromopropanoate
	Propionic acid, 2,3-dibromo-, methyl ester
Inchi:	InChI=1S/C4H6Br2O2/c1-8-4(7)3(6)2-5/h3H,2H2,1H3
InchiKey:	ROXQOUUAPQUMLN-UHFFFAOYSA-N
Formula:	C4H6Br2O2
SMILES:	COC(=O)C(Br)CBr
Mol. weight [g/mol]:	245.90
CAS:	1729-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-224.92	kJ/mol	Joback Method
hf	-323.31	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	46.14	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.318		Crippen Method
mcvol	109.660	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1070.00		NIST Webbook
tb	499.09	K	Joback Method
tc	720.07	K	Joback Method
tf	311.60	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	186.60	J/mol×K	499.09	Joback Method
cpg	217.73	J/mol×K	683.24	Joback Method
cpg	212.25	J/mol×K	646.41	Joback Method
cpg	206.40	J/mol×K	609.58	Joback Method
cpg	200.19	J/mol×K	572.75	Joback Method
cpg	193.59	J/mol×K	535.92	Joback Method
cpg	222.87	J/mol×K	720.07	Joback Method
dvisc	0.0003676	Pa×s	499.09	Joback Method
dvisc	0.0004592	Pa×s	467.84	Joback Method
dvisc	0.0005922	Pa×s	436.59	Joback Method
dvisc	0.0007943	Pa×s	405.35	Joback Method
dvisc	0.0011189	Pa×s	374.10	Joback Method
dvisc	0.0016778	Pa×s	342.85	Joback Method
dvisc	0.0027287	Pa×s	311.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1729675&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume