Propanedioic acid, bromo-, dimethyl ester

Other names: 2-Bromo dimethyl malonate
Dimethyl bromomalonate
Inchi: InChI=1S/C5H7BrO4/c1-9-4(7)3(6)5(8)10-2/h3H,1-2H3
InchiKey: NEMOJKROKMMQBQ-UHFFFAOYSA-N
Formula: C5H7BrO4
SMILES: COC(=O)C(Br)C(=O)OC
Mol. weight [g/mol]: 211.01
CAS: 868-26-8

Physical Properties

Property code	Value	Unit	Source
gf	-464.74	kJ/mol	Joback Method
hf	-615.08	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	51.08	kJ/mol	Joback Method
log10ws	-0.18		Crippen Method
logp	0.096		Crippen Method
mcvol	113.690	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	532.10	K	Joback Method
tc	741.52	K	Joback Method
tf	335.23	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.92	J/mol×K	532.10	Joback Method
cpg	234.93	J/mol×K	567.00	Joback Method
cpg	242.59	J/mol×K	601.91	Joback Method
cpg	249.90	J/mol×K	636.81	Joback Method
cpg	256.83	J/mol×K	671.71	Joback Method
cpg	263.39	J/mol×K	706.62	Joback Method
cpg	269.56	J/mol×K	741.52	Joback Method

dvisc	0.0021960	Pa×s	335.23	Joback Method
dvisc	0.0013461	Pa×s	368.04	Joback Method
dvisc	0.0008939	Pa×s	400.85	Joback Method
dvisc	0.0006316	Pa×s	433.67	Joback Method
dvisc	0.0004686	Pa×s	466.48	Joback Method
dvisc	0.0003616	Pa×s	499.29	Joback Method
dvisc	0.0002881	Pa×s	532.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.70	K	1.50	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=C868268&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume