Propanedioic acid, bromo-, diethyl ester

Other names:	Bromomalonic acid diethyl ester
	Diethyl 2-bromomalonate
	Diethyl «alpha»-bromomalonate
	Ethyl bromomalonate
	diethyl bromomalonate
	malonic acid, bromo-, diethyl ester
	«alpha»-Bromomalonic ester
Inchi:	InChI=1S/C7H11BrO4/c1-3-11-6(9)5(8)7(10)12-4-2/h5H,3-4H2,1-2H3
InchiKey:	FNJVDWXUKLTFFL-UHFFFAOYSA-N
Formula:	C7H11BrO4
SMILES:	CCOC(=O)C(Br)C(=O)OCC
Mol. weight [g/mol]:	239.06
CAS:	685-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-447.90	kJ/mol	Joback Method
hf	-656.36	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	0.876		Crippen Method
mcvol	141.870	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	507.20	K	NIST Webbook
tc	780.93	K	Joback Method
tf	357.77	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.59	J/mol×K	577.86	Joback Method
cpg	359.83	J/mol×K	747.08	Joback Method

cpg	351.58	J/mol×K	713.24	Joback Method
cpg	342.82	J/mol×K	679.39	Joback Method
cpg	333.57	J/mol×K	645.55	Joback Method
cpg	323.82	J/mol×K	611.70	Joback Method
cpg	367.58	J/mol×K	780.93	Joback Method
dvisc	0.0002309	Pa×s	577.86	Joback Method
dvisc	0.0002929	Pa×s	541.18	Joback Method
dvisc	0.0003847	Pa×s	504.50	Joback Method
dvisc	0.0005273	Pa×s	467.81	Joback Method
dvisc	0.0007626	Pa×s	431.13	Joback Method
dvisc	0.0011813	Pa×s	394.45	Joback Method
dvisc	0.0020016	Pa×s	357.77	Joback Method

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
303.15	101.30	0.0036140

Reference *https://www.doi.org/10.1016/j.tca.2004.07.014*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C685870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Speeds of sound, isentropic compressibilities, viscosities, and excess molar volumes of binary mixtures of alkanoates with tetra- and trichloromethanes at 303.15 K:	https://www.doi.org/10.1016/j.tca.2004.07.014
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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