Propanoic acid, 2,3-dibromo-, ethyl ester

Other names:	Ethyl 2,3-dibromopropionate
	Ethyl «alpha»,«beta»-dibromopropionate
	Propionic acid, 2,3-dibromo-, ethyl ester
Inchi:	InChI=1S/C5H8Br2O2/c1-2-9-5(8)4(7)3-6/h4H,2-3H2,1H3
InchiKey:	OENICUBCLXKLJQ-UHFFFAOYSA-N
Formula:	C5H8Br2O2
SMILES:	CCOC(=O)C(Br)CBr
Mol. weight [g/mol]:	259.92
CAS:	3674-13-3

Physical Properties

Property code	Value	Unit	Source
gf	-216.50	kJ/mol	Joback Method
hf	-343.95	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.708		Crippen Method
mcvol	123.750	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
tb	521.97	K	Joback Method
tc	739.28	K	Joback Method
tf	322.87	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.54	J/mol×K	521.97	Joback Method
cpg	263.67	J/mol×K	703.06	Joback Method
cpg	257.11	J/mol×K	666.84	Joback Method
cpg	250.14	J/mol×K	630.63	Joback Method

cpg	242.73	J/mol×K	594.41	Joback Method
cpg	234.87	J/mol×K	558.19	Joback Method
cpg	269.82	J/mol×K	739.28	Joback Method
dvisc	0.0003296	Pa×s	521.97	Joback Method
dvisc	0.0004142	Pa×s	488.79	Joback Method
dvisc	0.0005381	Pa×s	455.60	Joback Method
dvisc	0.0007285	Pa×s	422.42	Joback Method
dvisc	0.0010386	Pa×s	389.24	Joback Method
dvisc	0.0015817	Pa×s	356.05	Joback Method
dvisc	0.0026265	Pa×s	322.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.70	K	99.50	NIST Webbook

Sources

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=C3674133&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume