Diethyl dibromomalonate

Other names:	Propanedioic acid, dibromo-, diethyl ester
	Ethyl dibromomalonate
	Malonic acid, dibromo-, diethyl ester
	Dibromo malonic acid, diethyl ester
Inchi:	InChI=1S/C7H10Br2O4/c1-3-12-5(10)7(8,9)6(11)13-4-2/h3-4H2,1-2H3
InchiKey:	PFZYFZRUPFUEOB-UHFFFAOYSA-N
Formula:	C7H10Br2O4
SMILES:	CCOC(=O)C(Br)(Br)C(=O)OCC
Mol. weight [g/mol]:	317.96
CAS:	631-22-1

Physical Properties

Property code	Value	Unit	Source
gf	-428.30	kJ/mol	Joback Method
hf	-633.50	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	61.06	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.599		Crippen Method
mcvol	159.370	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	641.23	K	Joback Method
tc	864.25	K	Joback Method
tf	434.99	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.53	J/mol×K	641.23	Joback Method
cpg	389.56	J/mol×K	827.08	Joback Method
cpg	382.58	J/mol×K	789.91	Joback Method
cpg	375.01	J/mol×K	752.74	Joback Method
cpg	366.83	J/mol×K	715.57	Joback Method

cpg	358.01	J/mol×K	678.40	Joback Method
cpg	395.99	J/mol×K	864.25	Joback Method
dvisc	0.0001854	Pa×s	641.23	Joback Method
dvisc	0.0002315	Pa×s	606.86	Joback Method
dvisc	0.0002970	Pa×s	572.48	Joback Method
dvisc	0.0003933	Pa×s	538.11	Joback Method
dvisc	0.0005411	Pa×s	503.74	Joback Method
dvisc	0.0007801	Pa×s	469.36	Joback Method
dvisc	0.0011915	Pa×s	434.99	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=C631221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.