Propanedioic acid, dibromo-, dimethyl ester

Other names: dimethyl dibromomalonate
Inchi: InChI=1S/C5H6Br2O4/c1-10-3(8)5(6,7)4(9)11-2/h1-2H3
InchiKey: UWZGBUTYDAIEAS-UHFFFAOYSA-N
Formula: C5H6Br2O4
SMILES: COC(=O)C(Br)(Br)C(=O)OC
Mol. weight [g/mol]: 289.91
CAS: 37167-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-445.14	kJ/mol	Joback Method
hf	-592.22	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.818		Crippen Method
mcvol	131.190	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
rinpol	1252.00		NIST Webbook
tb	595.47	K	Joback Method
tc	827.23	K	Joback Method
tf	412.45	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.13	J/mol×K	595.47	Joback Method
cpg	265.65	J/mol×K	634.10	Joback Method
cpg	272.60	J/mol×K	672.72	Joback Method
cpg	279.01	J/mol×K	711.35	Joback Method
cpg	284.90	J/mol×K	749.98	Joback Method
cpg	290.29	J/mol×K	788.60	Joback Method
cpg	295.21	J/mol×K	827.23	Joback Method

dvisc	0.0014055	Pa×s	412.45	Joback Method
dvisc	0.0009529	Pa×s	442.95	Joback Method
dvisc	0.0006792	Pa×s	473.46	Joback Method
dvisc	0.0005044	Pa×s	503.96	Joback Method
dvisc	0.0003875	Pa×s	534.46	Joback Method
dvisc	0.0003063	Pa×s	564.97	Joback Method
dvisc	0.0002480	Pa×s	595.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37167592&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