Propanedioic acid, oxo-, bis(2-methylpropyl) ester

Other names: Mesoxalic acid, diisobutyl ester
Inchi: InChI=1S/C11H18O5/c1-7(2)5-15-10(13)9(12)11(14)16-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey: KTQZIUYTZLTGJE-UHFFFAOYSA-N
Formula: C11H18O5
SMILES: CC(C)COC(=O)C(=O)C(=O)OCC(C)C
Mol. weight [g/mol]: 230.26
CAS: 92778-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-559.90	kJ/mol	Joback Method
hf	-883.11	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	0.954		Crippen Method
mcvol	182.300	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
tb	656.65	K	Joback Method
tc	848.84	K	Joback Method
tf	377.98	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.23	J/mol×K	656.65	Joback Method
cpg	545.21	J/mol×K	816.81	Joback Method
cpg	534.62	J/mol×K	784.78	Joback Method
cpg	523.33	J/mol×K	752.75	Joback Method
cpg	511.33	J/mol×K	720.71	Joback Method
cpg	498.63	J/mol×K	688.68	Joback Method
cpg	555.08	J/mol×K	848.84	Joback Method
dvisc	0.0001473	Pa×s	656.65	Joback Method

dvisc	0.0001947	Pa×s	610.20	Joback Method
dvisc	0.0002693	Pa×s	563.76	Joback Method
dvisc	0.0003950	Pa×s	517.32	Joback Method
dvisc	0.0006248	Pa×s	470.87	Joback Method
dvisc	0.0010925	Pa×s	424.43	Joback Method
dvisc	0.0021916	Pa×s	377.98	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=C92778433&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