

Propanedioic acid, oxo-, bis(1-methylethyl) ester

Inchi:	InChI=1S/C9H14O5/c1-5(2)13-8(11)7(10)9(12)14-6(3)4/h5-6H,1-4H3
InchiKey:	ISAKWFYKUTYAQE-UHFFFAOYSA-N
Formula:	C9H14O5
SMILES:	CC(C)OC(=O)C(=O)C(=O)OC(C)C
Mol. weight [g/mol]:	202.20
CAS:	73972-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-576.74	kJ/mol	Joback Method
hf	-841.83	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.459		Crippen Method
mcvol	154.120	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	610.89	K	Joback Method
tc	807.59	K	Joback Method
tf	355.44	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.81	J/molxK	610.89	Joback Method
cpg	440.03	J/molxK	774.80	Joback Method
cpg	430.41	J/molxK	742.02	Joback Method
cpg	420.16	J/molxK	709.24	Joback Method
cpg	409.31	J/molxK	676.46	Joback Method
cpg	397.85	J/molxK	643.67	Joback Method
cpg	449.04	J/molxK	807.59	Joback Method
dvisc	0.0001862	Paxs	610.89	Joback Method
dvisc	0.0002443	Paxs	568.32	Joback Method

dvisc	0.0003351	Paxs	525.74	Joback Method
dvisc	0.0004858	Paxs	483.17	Joback Method
dvisc	0.0007567	Paxs	440.59	Joback Method
dvisc	0.0012961	Paxs	398.02	Joback Method
dvisc	0.0025252	Paxs	355.44	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=C73972391&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

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