Malonic aicd,[(carboxyamino)oxy]-, triethyl ester

Inchi: InChI=1S/C10H17NO7/c1-4-15-8(12)7(9(13)16-5-2)18-11-10(14)17-6-3/h7H,4-6H2,1-3H

InchiKey: MLCVSERZZDBICP-UHFFFAOYSA-N

Formula: C10H17NO7

SMILES: CCOC(=O)C(ON=C(O)OCC)C(=O)OCC

Mol. weight [g/mol]: 263.24

Physical Properties

Property code	Value	Unit	Source
hf	-1088.85	kJ/mol	Joback Method
hvap	80.67	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.363		Crippen Method
mcvol	189.930	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
tb	793.92	K	Joback Method
tc	987.31	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009217&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

hf: Enthalpy of formation 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

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