Triethyl (1z)-1-propene-1,2,3-tricarboxylate

Inchi: InChI=1S/C12H18O6/c1-4-16-10(13)7-9(12(15)18-6-3)8-11(14)17-5-2/h7H,4-6,8H2,1-3H
InchiKey: IDDWGDKSBYYEPL-CLFYSBASSA-N
Formula: C12H18O6
SMILES: CCOC(=O)C=C(CC(=O)OCC)C(=O)OCC
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-579.93	kJ/mol	Joback Method
hf	-917.98	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.992		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
tb	706.87	K	Joback Method
tc	899.36	K	Joback Method
tf	422.44	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.23	J/mol×K	706.87	Joback Method
cpg	552.13	J/mol×K	738.95	Joback Method
cpg	564.31	J/mol×K	771.03	Joback Method
cpg	575.76	J/mol×K	803.11	Joback Method
cpg	586.49	J/mol×K	835.20	Joback Method
cpg	596.50	J/mol×K	867.28	Joback Method
cpg	605.78	J/mol×K	899.36	Joback Method

Sources

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=B6009419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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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