2,4,6-tris-(Methoxycarbonyl)-1-hexene

Inchi: InChI=1S/C12H18O6/c1-8(11(14)17-3)7-9(12(15)18-4)5-6-10(13)16-2/h9H,1,5-7H2,2-4H
InchiKey: ROTVGWWUMVNODQ-UHFFFAOYSA-N
Formula: C12H18O6
SMILES: C=C(CC(CCC(=O)OC)C(=O)OC)C(=O)OC
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-574.75	kJ/mol	Joback Method
hf	-915.05	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	68.80	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.848		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	698.95	K	Joback Method
tc	890.93	K	Joback Method
tf	410.76	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.39	J/mol×K	698.95	Joback Method
cpg	552.48	J/mol×K	730.95	Joback Method
cpg	564.84	J/mol×K	762.94	Joback Method
cpg	576.46	J/mol×K	794.94	Joback Method
cpg	587.32	J/mol×K	826.94	Joback Method
cpg	597.43	J/mol×K	858.94	Joback Method
cpg	606.77	J/mol×K	890.93	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=R582177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume