1,2,3-Propenetricarboxylic acid, tris(1-methylpropyl) ester

Other names: Tri(sec-butyl) (1z)-1-propene-1,2,3-tricarboxylate
Inchi: InChI=1S/C18H30O6/c1-7-12(4)22-16(19)10-15(18(21)24-14(6)9-3)11-17(20)23-13(5)8-2
InchiKey: RNKDXUCWFNMDKW-GDNBJRDFSA-N
Formula: C18H30O6
SMILES: CCC(C)OC(=O)C=C(CC(=O)OC(C)CC)C(=O)OC(C)CC
Mol. weight [g/mol]: 342.43
CAS: 111530-50-8

Physical Properties

Property code	Value	Unit	Source
gf	-536.73	kJ/mol	Joback Method
hf	-1057.66	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.328		Crippen Method
mcvol	282.500	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
tb	842.83	K	Joback Method
tc	1040.87	K	Joback Method
tf	445.06	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.99	J/mol×K	842.83	Joback Method
cpg	892.55	J/mol×K	875.84	Joback Method
cpg	907.00	J/mol×K	908.84	Joback Method
cpg	920.36	J/mol×K	941.85	Joback Method
cpg	932.64	J/mol×K	974.86	Joback Method
cpg	943.86	J/mol×K	1007.87	Joback Method
cpg	954.03	J/mol×K	1040.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111530508&Units=SI

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