1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tripropyl ester

Other names: tripropyl citrate
Inchi: InChI=1S/C15H26O7/c1-4-7-20-12(16)10-15(19,14(18)22-9-6-3)11-13(17)21-8-5-2/h19H
InchiKey: ODHUFJLMXDXVRC-UHFFFAOYSA-N
Formula: C15H26O7
SMILES: CCCOC(=O)CC(O)(CC(=O)OCCC)C(=O)OCCC
Mol. weight [g/mol]: 318.36
CAS: 1587-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-760.32	kJ/mol	Joback Method
hf	-1248.31	kJ/mol	Joback Method
hfus	39.64	kJ/mol	Joback Method
hvap	91.83	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.357		Crippen Method
mcvol	250.400	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
tb	860.42	K	Joback Method
tc	1055.88	K	Joback Method
tf	538.53	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.65	J/mol×K	860.42	Joback Method
cpg	801.23	J/mol×K	893.00	Joback Method
cpg	812.86	J/mol×K	925.57	Joback Method
cpg	823.54	J/mol×K	958.15	Joback Method
cpg	833.28	J/mol×K	990.72	Joback Method
cpg	842.11	J/mol×K	1023.30	Joback Method
cpg	850.02	J/mol×K	1055.88	Joback Method
dvisc	0.0002599	Pa×s	538.53	Joback Method

dvisc	0.0001161	Pa×s	592.18	Joback Method
dvisc	0.0000593	Pa×s	645.83	Joback Method
dvisc	0.0000336	Pa×s	699.47	Joback Method
dvisc	0.0000206	Pa×s	753.12	Joback Method
dvisc	0.0000135	Pa×s	806.77	Joback Method
dvisc	0.0000093	Pa×s	860.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1587219&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

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