1,2,3-Propanetricarboxylic acid, 2-acetoxy-, tri(4-methylpentyl) ester

Inchi: InChI=1S/C26H46O8/c1-19(2)11-8-14-31-23(28)17-26(34-22(7)27,25(30)33-16-10-13-21
InchiKey: KTWCWRHURMHPCW-UHFFFAOYSA-N
Formula: C26H46O8
SMILES: CC(=O)OC(CC(=O)OCCCC(C)C)(CC(=O)OCCCC(C)C)C(=O)OCCCC(C)C
Mol. weight [g/mol]: 486.64
CAS: 85261-16-1

Physical Properties

Property code	Value	Unit	Source
gf	-772.12	kJ/mol	Joback Method
hf	-1583.76	kJ/mol	Joback Method
hfus	56.26	kJ/mol	Joback Method
hvap	107.63	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.007		Crippen Method
mcvol	406.960	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
tb	1094.89	K	Joback Method
tc	1356.80	K	Joback Method
tf	628.84	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.64	J/mol×K	1094.89	Joback Method
cpg	1447.78	J/mol×K	1138.54	Joback Method
cpg	1459.39	J/mol×K	1182.19	Joback Method
cpg	1468.52	J/mol×K	1225.84	Joback Method
cpg	1475.21	J/mol×K	1269.50	Joback Method
cpg	1479.54	J/mol×K	1313.15	Joback Method
cpg	1481.55	J/mol×K	1356.80	Joback Method
dvisc	0.0001210	Pa×s	628.84	Joback Method
dvisc	0.0000543	Pa×s	706.51	Joback Method

dvisc	0.0000285	Pa×s	784.19	Joback Method
dvisc	0.0000168	Pa×s	861.87	Joback Method
dvisc	0.0000108	Pa×s	939.54	Joback Method
dvisc	0.0000075	Pa×s	1017.21	Joback Method
dvisc	0.0000054	Pa×s	1094.89	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=C85261161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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