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

Inchi: InChI=1S/C24H44O7/c1-4-7-10-13-16-29-21(25)19-24(28,23(27)31-18-15-12-9-6-3)20-2

InchiKey: AMMPRZCMKXDUNE-UHFFFAOYSA-N

Formula: C24H44O7

SMILES: CCCCCCOC(=O)CC(O)(CC(=O)OCCCCCC)C(=O)OCCCCCC

Mol. weight [g/mol]: 444.60

CAS: 16544-70-0

Physical Properties

Property code	Value	Unit	Source
gf	-684.54	kJ/mol	Joback Method
hf	-1434.07	kJ/mol	Joback Method
hfus	62.95	kJ/mol	Joback Method
hvap	111.87	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.868		Crippen Method
mcvol	377.210	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
tb	1066.34	K	Joback Method
tc	1331.50	K	Joback Method
tf	639.96	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1329.05	J/mol×K	1066.34	Joback Method
cpg	1345.48	J/mol×K	1110.53	Joback Method
cpg	1359.77	J/mol×K	1154.73	Joback Method
cpg	1372.00	J/mol×K	1198.92	Joback Method
cpg	1382.28	J/mol×K	1243.12	Joback Method
cpg	1390.67	J/mol×K	1287.31	Joback Method
cpg	1397.27	J/mol×K	1331.50	Joback Method
dvisc	0.0000556	Pa×s	639.96	Joback Method
dvisc	0.0000231	Pa×s	711.02	Joback Method

dvisc	0.0000112	Pa×s	782.09	Joback Method
dvisc	0.0000062	Pa×s	853.15	Joback Method
dvisc	0.0000037	Pa×s	924.21	Joback Method
dvisc	0.0000024	Pa×s	995.28	Joback Method
dvisc	0.0000016	Pa×s	1066.34	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=C16544700&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
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