Diglycolic acid, hexyl propyl ester

Inchi: InChI=1S/C13H24O5/c1-3-5-6-7-9-18-13(15)11-16-10-12(14)17-8-4-2/h3-11H2,1-2H3
InchiKey: BTHOZQCNZRWUIA-UHFFFAOYSA-N
Formula: C13H24O5
SMILES: CCCCCCOC(=O)COCC(=O)OCCC
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
gf	-514.26	kJ/mol	Joback Method
hf	-933.47	kJ/mol	Joback Method
hfus	36.19	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.080		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	671.84	K	Joback Method
tc	848.38	K	Joback Method
tf	402.82	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.49	J/mol×K	671.84	Joback Method
cpg	611.45	J/mol×K	701.26	Joback Method
cpg	625.72	J/mol×K	730.69	Joback Method
cpg	639.30	J/mol×K	760.11	Joback Method
cpg	652.19	J/mol×K	789.54	Joback Method
cpg	664.37	J/mol×K	818.96	Joback Method
cpg	675.85	J/mol×K	848.38	Joback Method
dvisc	0.0011295	Pa×s	402.82	Joback Method

dvisc	0.0006229	Pa×s	447.66	Joback Method
dvisc	0.0003829	Pa×s	492.49	Joback Method
dvisc	0.0002553	Pa×s	537.33	Joback Method
dvisc	0.0001811	Pa×s	582.17	Joback Method
dvisc	0.0001350	Pa×s	627.00	Joback Method
dvisc	0.0001046	Pa×s	671.84	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=U382055&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume