Diglycolic acid, di(hexyl) ester

Other names: dihexyl 2,2'-oxydiacetate
dihexyl diglycolate
Inchi: InChI=1S/C16H30O5/c1-3-5-7-9-11-20-15(17)13-19-14-16(18)21-12-10-8-6-4-2/h3-14H2
InchiKey: HFMKUFQIARQMBH-UHFFFAOYSA-N
Formula: C16H30O5
SMILES: CCCCCCOC(=O)COCC(=O)OCCCCCC
Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-489.00	kJ/mol	Joback Method
hf	-995.39	kJ/mol	Joback Method
hfus	43.96	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.250		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	740.48	K	Joback Method
tc	918.04	K	Joback Method
tf	436.63	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.64	J/mol×K	740.48	Joback Method
cpg	780.01	J/mol×K	770.07	Joback Method
cpg	795.54	J/mol×K	799.67	Joback Method
cpg	810.22	J/mol×K	829.26	Joback Method
cpg	824.05	J/mol×K	858.86	Joback Method
cpg	837.03	J/mol×K	888.45	Joback Method

cpg	849.16	J/mol×K	918.04	Joback Method
dvisc	0.0008707	Pa×s	436.63	Joback Method
dvisc	0.0004605	Pa×s	487.27	Joback Method
dvisc	0.0002746	Pa×s	537.91	Joback Method
dvisc	0.0001790	Pa×s	588.56	Joback Method
dvisc	0.0001249	Pa×s	639.20	Joback Method
dvisc	0.0000918	Pa×s	689.84	Joback Method
dvisc	0.0000704	Pa×s	740.48	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=U382059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
New Highly CO2-Philic Diglycolic Acid Esters: Synthesis and Solubility in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je900893e

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