Diglycolic acid, hexyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C18H34O5/c1-6-7-8-9-10-22-16(19)13-21-14-17(20)23-12-15(2)11-18(3,4)5/h1

InchiKey: JODLFGWCCUEJEX-UHFFFAOYSA-N

Formula: C18H34O5

SMILES: CCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	-471.76	kJ/mol	Joback Method
hf	-1050.70	kJ/mol	Joback Method
hfus	38.20	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.742		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	782.57	K	Joback Method
tc	968.21	K	Joback Method
tf	446.59	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.32	J/mol×K	782.57	Joback Method
cpg	899.73	J/mol×K	813.51	Joback Method
cpg	916.11	J/mol×K	844.45	Joback Method
cpg	931.48	J/mol×K	875.39	Joback Method
cpg	945.86	J/mol×K	906.33	Joback Method
cpg	959.26	J/mol×K	937.27	Joback Method
cpg	971.71	J/mol×K	968.21	Joback Method
dvisc	0.0008126	Pa×s	446.59	Joback Method

dvisc	0.0003710	Pa×s	502.59	Joback Method
dvisc	0.0001983	Pa×s	558.58	Joback Method
dvisc	0.0001187	Pa×s	614.58	Joback Method
dvisc	0.0000775	Pa×s	670.58	Joback Method
dvisc	0.0000540	Pa×s	726.57	Joback Method
dvisc	0.0000396	Pa×s	782.57	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=U382041&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