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

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

InchiKey: YMPKDSARQHHRRL-UHFFFAOYSA-N

Formula: C18H34O5

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

Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	-474.20	kJ/mol	Joback Method
hf	-1055.98	kJ/mol	Joback Method
hfus	34.68	kJ/mol	Joback Method
hvap	74.31	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.598		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	782.13	K	Joback Method
tc	969.34	K	Joback Method
tf	431.59	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.81	J/mol×K	782.13	Joback Method
cpg	960.27	J/mol×K	938.14	Joback Method
cpg	946.82	J/mol×K	906.94	Joback Method
cpg	932.36	J/mol×K	875.74	Joback Method
cpg	916.89	J/mol×K	844.53	Joback Method
cpg	900.38	J/mol×K	813.33	Joback Method
cpg	972.74	J/mol×K	969.34	Joback Method
dvisc	0.0000365	Pa×s	782.13	Joback Method

dvisc	0.0000506	Pa×s	723.71	Joback Method
dvisc	0.0000745	Pa×s	665.28	Joback Method
dvisc	0.0001180	Pa×s	606.86	Joback Method
dvisc	0.0002061	Pa×s	548.44	Joback Method
dvisc	0.0004116	Pa×s	490.01	Joback Method
dvisc	0.0009908	Pa×s	431.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382040&Units=SI

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