Diglycolic acid, isohexyl 2-methylbutyl ester

Inchi: InChI=1S/C15H28O5/c1-5-13(4)9-20-15(17)11-18-10-14(16)19-8-6-7-12(2)3/h12-13H,5-1
InchiKey: AHUIXQXHCCAIBN-UHFFFAOYSA-N
Formula: C15H28O5
SMILES: CCC(C)COC(=O)COCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
gf	-502.30	kJ/mol	Joback Method
hf	-985.31	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.572		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	716.72	K	Joback Method
tc	897.37	K	Joback Method
tf	395.36	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.73	J/mol×K	716.72	Joback Method
cpg	780.93	J/mol×K	867.26	Joback Method
cpg	767.99	J/mol×K	837.15	Joback Method
cpg	754.19	J/mol×K	807.05	Joback Method
cpg	739.55	J/mol×K	776.94	Joback Method
cpg	724.06	J/mol×K	746.83	Joback Method
cpg	793.03	J/mol×K	897.37	Joback Method
dvisc	0.0000689	Pa×s	716.72	Joback Method

dvisc	0.0000929	Pa×s	663.16	Joback Method
dvisc	0.0001321	Pa×s	609.60	Joback Method
dvisc	0.0002010	Pa×s	556.04	Joback Method
dvisc	0.0003346	Pa×s	502.48	Joback Method
dvisc	0.0006288	Pa×s	448.92	Joback Method
dvisc	0.0014019	Pa×s	395.36	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=U381815&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