Diglycolic acid, ethyl 3-methylpent-2-yl ester

Inchi: InChI=1S/C12H22O5/c1-5-9(3)10(4)17-12(14)8-15-7-11(13)16-6-2/h9-10H,5-8H2,1-4H3
InchiKey: WAUIMLYYOVTFTJ-UHFFFAOYSA-N
Formula: C12H22O5
SMILES: CCOC(=O)COCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
gf	-527.56	kJ/mol	Joback Method
hf	-923.39	kJ/mol	Joback Method
hfus	26.55	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.544		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1925.00		NIST Webbook
tb	648.08	K	Joback Method
tc	830.65	K	Joback Method
tf	361.55	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.21	J/mol×K	648.08	Joback Method
cpg	611.82	J/mol×K	800.22	Joback Method
cpg	599.71	J/mol×K	769.79	Joback Method
cpg	586.88	J/mol×K	739.36	Joback Method
cpg	573.35	J/mol×K	708.94	Joback Method
cpg	559.13	J/mol×K	678.51	Joback Method
cpg	623.21	J/mol×K	830.65	Joback Method
dvisc	0.0001023	Pa×s	648.08	Joback Method
dvisc	0.0001370	Pa×s	600.32	Joback Method

dvisc	0.0001928	Pa×s	552.57	Joback Method
dvisc	0.0002895	Pa×s	504.81	Joback Method
dvisc	0.0004732	Pa×s	457.06	Joback Method
dvisc	0.0008676	Pa×s	409.31	Joback Method
dvisc	0.0018669	Pa×s	361.55	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=U381869&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