Diglycolic acid, ethyl isobutyl ester

Inchi: InChI=1S/C10H18O5/c1-4-14-9(11)6-13-7-10(12)15-5-8(2)3/h8H,4-7H2,1-3H3
InchiKey: MHJYPHKVVMLGGZ-UHFFFAOYSA-N
Formula: C10H18O5
SMILES: CCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-541.96	kJ/mol	Joback Method
hf	-876.83	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-0.58		Crippen Method
logp	0.765		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1727.00		NIST Webbook
tb	602.76	K	Joback Method
tc	785.24	K	Joback Method
tf	354.01	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.75	J/mol×K	602.76	Joback Method
cpg	455.10	J/mol×K	633.17	Joback Method
cpg	467.90	J/mol×K	663.59	Joback Method
cpg	480.14	J/mol×K	694.00	Joback Method
cpg	491.81	J/mol×K	724.41	Joback Method
cpg	502.89	J/mol×K	754.83	Joback Method
cpg	513.38	J/mol×K	785.24	Joback Method
dvisc	0.0017099	Pa×s	354.01	Joback Method
dvisc	0.0009050	Pa×s	395.47	Joback Method

dvisc	0.0005405	Pa×s	436.93	Joback Method
dvisc	0.0003529	Pa×s	478.38	Joback Method
dvisc	0.0002467	Pa×s	519.84	Joback Method
dvisc	0.0001818	Pa×s	561.30	Joback Method
dvisc	0.0001397	Pa×s	602.76	Joback Method

Sources

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=U382123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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