Diglycolic acid, ethyl 2-methylpentyl ester

Inchi: InChI=1S/C12H22O5/c1-4-6-10(3)7-17-12(14)9-15-8-11(13)16-5-2/h10H,4-9H2,1-3H3
InchiKey: PCKMDQGHVBYEAB-UHFFFAOYSA-N
Formula: C12H22O5
SMILES: CCCC(C)COC(=O)COCC(=O)OCC
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
gf	-525.12	kJ/mol	Joback Method
hf	-918.11	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.545		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook
tb	648.52	K	Joback Method
tc	828.30	K	Joback Method
tf	376.55	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.76	J/mol×K	648.52	Joback Method
cpg	558.41	J/mol×K	678.48	Joback Method
cpg	572.40	J/mol×K	708.45	Joback Method
cpg	585.72	J/mol×K	738.41	Joback Method
cpg	598.37	J/mol×K	768.38	Joback Method
cpg	610.34	J/mol×K	798.34	Joback Method
cpg	621.62	J/mol×K	828.30	Joback Method
dvisc	0.0014862	Pa×s	376.55	Joback Method

dvisc	0.0007629	Pa×s	421.88	Joback Method
dvisc	0.0004458	Pa×s	467.21	Joback Method
dvisc	0.0002864	Pa×s	512.53	Joback Method
dvisc	0.0001977	Pa×s	557.86	Joback Method
dvisc	0.0001443	Pa×s	603.19	Joback Method
dvisc	0.0001101	Pa×s	648.52	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=U381792&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