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

Inchi: InChI=1S/C13H24O5/c1-5-7-17-12(14)8-16-9-13(15)18-11(4)10(3)6-2/h10-11H,5-9H2,1-
InchiKey: QMVCZQAADRDHAJ-UHFFFAOYSA-N
Formula: C13H24O5
SMILES: CCCOC(=O)COCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
gf	-519.14	kJ/mol	Joback Method
hf	-944.03	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.934		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	670.96	K	Joback Method
tc	852.46	K	Joback Method
tf	372.82	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.43	J/mol×K	670.96	Joback Method
cpg	612.87	J/mol×K	701.21	Joback Method
cpg	627.57	J/mol×K	731.46	Joback Method
cpg	641.52	J/mol×K	761.71	Joback Method
cpg	654.72	J/mol×K	791.96	Joback Method
cpg	667.17	J/mol×K	822.21	Joback Method
cpg	678.85	J/mol×K	852.46	Joback Method
dvisc	0.0017069	Pa×s	372.82	Joback Method

dvisc	0.0007834	Pa×s	422.51	Joback Method
dvisc	0.0004236	Pa×s	472.20	Joback Method
dvisc	0.0002575	Pa×s	521.89	Joback Method
dvisc	0.0001707	Pa×s	571.58	Joback Method
dvisc	0.0001208	Pa×s	621.27	Joback Method
dvisc	0.0000900	Pa×s	670.96	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=U381870&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