Diglycolic acid, isobutyl neopentyl ester

Inchi: InChI=1S/C13H24O5/c1-10(2)6-17-11(14)7-16-8-12(15)18-9-13(3,4)5/h10H,6-9H2,1-5H3
InchiKey: JWUXQOVRODNNGU-UHFFFAOYSA-N
Formula: C13H24O5
SMILES: CC(C)COC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
gf	-513.86	kJ/mol	Joback Method
hf	-947.50	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	63.57	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.791		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	668.17	K	Joback Method
tc	854.57	K	Joback Method
tf	390.24	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.63	J/mol×K	668.17	Joback Method
cpg	615.26	J/mol×K	699.24	Joback Method
cpg	630.08	J/mol×K	730.30	Joback Method
cpg	644.10	J/mol×K	761.37	Joback Method
cpg	657.32	J/mol×K	792.44	Joback Method
cpg	669.74	J/mol×K	823.51	Joback Method
cpg	681.38	J/mol×K	854.57	Joback Method
dvisc	0.0014313	Pa×s	390.24	Joback Method

dvisc	0.0006922	Pa×s	436.56	Joback Method
dvisc	0.0003849	Pa×s	482.88	Joback Method
dvisc	0.0002371	Pa×s	529.21	Joback Method
dvisc	0.0001580	Pa×s	575.53	Joback Method
dvisc	0.0001118	Pa×s	621.85	Joback Method
dvisc	0.0000830	Pa×s	668.17	Joback Method

Sources

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=U381915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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