Diglycolic acid, isobutyl propyl ester

Inchi: InChI=1S/C11H20O5/c1-4-5-15-10(12)7-14-8-11(13)16-6-9(2)3/h9H,4-8H2,1-3H3
InchiKey: XYDWJMHQWBOITH-UHFFFAOYSA-N
Formula: C11H20O5
SMILES: CCCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]: 232.27

Physical Properties

Property code	Value	Unit	Source
gf	-533.54	kJ/mol	Joback Method
hf	-897.47	kJ/mol	Joback Method
hfus	27.48	kJ/mol	Joback Method
hvap	60.41	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	1.155		Crippen Method
mcvol	186.600	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	625.64	K	Joback Method
tc	806.61	K	Joback Method
tf	365.28	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.99	J/mol×K	625.64	Joback Method
cpg	506.03	J/mol×K	655.80	Joback Method
cpg	519.46	J/mol×K	685.96	Joback Method
cpg	532.28	J/mol×K	716.13	Joback Method
cpg	544.48	J/mol×K	746.29	Joback Method
cpg	556.04	J/mol×K	776.45	Joback Method
cpg	566.96	J/mol×K	806.61	Joback Method
dvisc	0.0016004	Pa×s	365.28	Joback Method

dvisc	0.0008339	Pa×s	408.67	Joback Method
dvisc	0.0004924	Pa×s	452.07	Joback Method
dvisc	0.0003189	Pa×s	495.46	Joback Method
dvisc	0.0002215	Pa×s	538.85	Joback Method
dvisc	0.0001624	Pa×s	582.25	Joback Method
dvisc	0.0001243	Pa×s	625.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382124&Units=SI
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

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