Diglycolic acid, isohexyl undecyl ester

Inchi: InChI=1S/C21H40O5/c1-4-5-6-7-8-9-10-11-12-15-25-20(22)17-24-18-21(23)26-16-13-14
InchiKey: PRDHQPSUWVGOCW-UHFFFAOYSA-N
Formula: C21H40O5
SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 372.54

Physical Properties

Property code	Value	Unit	Source
gf	-449.34	kJ/mol	Joback Method
hf	-1103.87	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.056		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	3101.00		NIST Webbook
rinpol	3101.00		NIST Webbook
tb	854.44	K	Joback Method
tc	1046.32	K	Joback Method
tf	477.98	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.62	J/mol×K	854.44	Joback Method
cpg	1142.77	J/mol×K	1014.34	Joback Method
cpg	1129.16	J/mol×K	982.36	Joback Method
cpg	1114.36	J/mol×K	950.38	Joback Method
cpg	1098.34	J/mol×K	918.40	Joback Method
cpg	1081.09	J/mol×K	886.42	Joback Method
cpg	1155.19	J/mol×K	1046.32	Joback Method
dvisc	0.0000314	Pa×s	854.44	Joback Method

dvisc	0.0000422	Pa×s	791.70	Joback Method
dvisc	0.0000597	Pa×s	728.95	Joback Method
dvisc	0.0000901	Pa×s	666.21	Joback Method
dvisc	0.0001480	Pa×s	603.47	Joback Method
dvisc	0.0002731	Pa×s	540.72	Joback Method
dvisc	0.0005916	Pa×s	477.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381865&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