Diglycolic acid, butyl hexyl ester

Inchi: InChI=1S/C14H26O5/c1-3-5-7-8-10-19-14(16)12-17-11-13(15)18-9-6-4-2/h3-12H2,1-2H3
InchiKey: XSDYSVQGKHJTQP-UHFFFAOYSA-N
Formula: C14H26O5
SMILES: CCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	-505.84	kJ/mol	Joback Method
hf	-954.11	kJ/mol	Joback Method
hfus	38.78	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.470		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	694.72	K	Joback Method
tc	871.11	K	Joback Method
tf	414.09	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.00	J/mol×K	694.72	Joback Method
cpg	666.47	J/mol×K	724.12	Joback Method
cpg	681.20	J/mol×K	753.52	Joback Method
cpg	695.18	J/mol×K	782.91	Joback Method
cpg	708.43	J/mol×K	812.31	Joback Method
cpg	720.92	J/mol×K	841.71	Joback Method
cpg	732.66	J/mol×K	871.11	Joback Method
dvisc	0.0010418	Pa×s	414.09	Joback Method

dvisc	0.0005663	Pa×s	460.86	Joback Method
dvisc	0.0003444	Pa×s	507.63	Joback Method
dvisc	0.0002278	Pa×s	554.40	Joback Method
dvisc	0.0001607	Pa×s	601.18	Joback Method
dvisc	0.0001192	Pa×s	647.95	Joback Method
dvisc	0.0000920	Pa×s	694.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382056&Units=SI

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