Diglycolic acid, hexyl 2-methylbutyl ester

Inchi: InChI=1S/C15H28O5/c1-4-6-7-8-9-19-14(16)11-18-12-15(17)20-10-13(3)5-2/h13H,4-12H
InchiKey: HQVCSQIYFUHCSW-UHFFFAOYSA-N
Formula: C15H28O5
SMILES: CCCCCCOC(=O)COCC(=O)OCC(C)CC
Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
gf	-499.86	kJ/mol	Joback Method
hf	-980.03	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.716		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	717.16	K	Joback Method
tc	895.78	K	Joback Method
tf	410.36	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.24	J/mol×K	717.16	Joback Method
cpg	723.36	J/mol×K	746.93	Joback Method
cpg	738.68	J/mol×K	776.70	Joback Method
cpg	753.17	J/mol×K	806.47	Joback Method
cpg	766.84	J/mol×K	836.24	Joback Method
cpg	779.69	J/mol×K	866.01	Joback Method
cpg	791.71	J/mol×K	895.78	Joback Method
dvisc	0.0011434	Pa×s	410.36	Joback Method

dvisc	0.0005637	Pa×s	461.49	Joback Method
dvisc	0.0003200	Pa×s	512.63	Joback Method
dvisc	0.0002013	Pa×s	563.76	Joback Method
dvisc	0.0001368	Pa×s	614.89	Joback Method
dvisc	0.0000986	Pa×s	666.03	Joback Method
dvisc	0.0000745	Pa×s	717.16	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=U381816&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