Diglycolic acid, pentyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C17H32O5/c1-6-7-8-9-21-15(18)12-20-13-16(19)22-11-14(2)10-17(3,4)5/h14H
InchiKey: MLMDXCIBAOURAE-UHFFFAOYSA-N
Formula: C17H32O5
SMILES: CCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 316.43

Physical Properties

Property code	Value	Unit	Source
gf	-480.18	kJ/mol	Joback Method
hf	-1030.06	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.352		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	759.69	K	Joback Method
tc	944.40	K	Joback Method
tf	435.32	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.69	J/mol×K	759.69	Joback Method
cpg	840.79	J/mol×K	790.47	Joback Method
cpg	856.91	J/mol×K	821.26	Joback Method
cpg	872.07	J/mol×K	852.04	Joback Method
cpg	886.28	J/mol×K	882.83	Joback Method
cpg	899.55	J/mol×K	913.61	Joback Method
cpg	911.90	J/mol×K	944.40	Joback Method
dvisc	0.0009176	Pa×s	435.32	Joback Method

dvisc	0.0004234	Pa×s	489.38	Joback Method
dvisc	0.0002278	Pa×s	543.44	Joback Method
dvisc	0.0001372	Pa×s	597.50	Joback Method
dvisc	0.0000898	Pa×s	651.57	Joback Method
dvisc	0.0000628	Pa×s	705.63	Joback Method
dvisc	0.0000462	Pa×s	759.69	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=U382039&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