Diglycolic acid, butyl 3-phenylpropyl ester

Inchi: InChI=1S/C17H24O5/c1-2-3-11-21-16(18)13-20-14-17(19)22-12-7-10-15-8-5-4-6-9-15/h4
InchiKey: BFNSTEKXYFTKGV-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CCCCOC(=O)COCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-368.17	kJ/mol	Joback Method
hf	-779.50	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.522		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook
tb	790.04	K	Joback Method
tc	989.47	K	Joback Method
tf	474.32	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.48	J/mol×K	790.04	Joback Method
cpg	748.59	J/mol×K	823.28	Joback Method
cpg	762.65	J/mol×K	856.52	Joback Method
cpg	775.65	J/mol×K	889.76	Joback Method
cpg	787.62	J/mol×K	922.99	Joback Method
cpg	798.55	J/mol×K	956.23	Joback Method
cpg	808.46	J/mol×K	989.47	Joback Method
dvisc	0.0006571	Pa×s	474.32	Joback Method

dvisc	0.0003642	Pa×s	526.94	Joback Method
dvisc	0.0002247	Pa×s	579.56	Joback Method
dvisc	0.0001502	Pa×s	632.18	Joback Method
dvisc	0.0001068	Pa×s	684.80	Joback Method
dvisc	0.0000798	Pa×s	737.42	Joback Method
dvisc	0.0000619	Pa×s	790.04	Joback Method

Sources

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=U382172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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