Diglycolic acid, phenethyl propyl ester

Inchi: InChI=1S/C15H20O5/c1-2-9-19-14(16)11-18-12-15(17)20-10-8-13-6-4-3-5-7-13/h3-7H,2,
InchiKey: XIUAEJOUYRVVNQ-UHFFFAOYSA-N
Formula: C15H20O5
SMILES: CCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 280.32

Physical Properties

Property code	Value	Unit	Source
gf	-385.01	kJ/mol	Joback Method
hf	-738.22	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	71.98	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.742		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	744.28	K	Joback Method
tc	945.99	K	Joback Method
tf	451.78	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.80	J/mol×K	744.28	Joback Method
cpg	636.35	J/mol×K	777.90	Joback Method
cpg	649.93	J/mol×K	811.52	Joback Method
cpg	662.54	J/mol×K	845.14	Joback Method
cpg	674.18	J/mol×K	878.75	Joback Method
cpg	684.87	J/mol×K	912.37	Joback Method
cpg	694.59	J/mol×K	945.99	Joback Method
dvisc	0.0007872	Pa×s	451.78	Joback Method

dvisc	0.0004480	Pa×s	500.53	Joback Method
dvisc	0.0002818	Pa×s	549.28	Joback Method
dvisc	0.0001911	Pa×s	598.03	Joback Method
dvisc	0.0001375	Pa×s	646.78	Joback Method
dvisc	0.0001035	Pa×s	695.53	Joback Method
dvisc	0.0000809	Pa×s	744.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382156&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