Diglycolic acid, isobutyl phenethyl ester

Inchi: InChI=1S/C16H22O5/c1-13(2)10-21-16(18)12-19-11-15(17)20-9-8-14-6-4-3-5-7-14/h3-7,
InchiKey: FFMVZFKFLQNJKN-UHFFFAOYSA-N
Formula: C16H22O5
SMILES: CC(C)COC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
gf	-379.03	kJ/mol	Joback Method
hf	-764.14	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.988		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	766.72	K	Joback Method
tc	969.72	K	Joback Method
tf	448.05	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.69	J/mol×K	766.72	Joback Method
cpg	692.74	J/mol×K	800.55	Joback Method
cpg	706.75	J/mol×K	834.39	Joback Method
cpg	719.71	J/mol×K	868.22	Joback Method
cpg	731.63	J/mol×K	902.05	Joback Method
cpg	742.52	J/mol×K	935.89	Joback Method
cpg	752.38	J/mol×K	969.72	Joback Method
dvisc	0.0008347	Pa×s	448.05	Joback Method

dvisc	0.0004359	Pa×s	501.16	Joback Method
dvisc	0.0002578	Pa×s	554.27	Joback Method
dvisc	0.0001671	Pa×s	607.38	Joback Method
dvisc	0.0001162	Pa×s	660.50	Joback Method
dvisc	0.0000852	Pa×s	713.61	Joback Method
dvisc	0.0000653	Pa×s	766.72	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=U382157&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